E. T. WHITTAKER'S QUANTUM FORMALISM

Forgotten precursor of Schwinger's variational principle

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Introduction. Edmond Taylor Whittaker (1873–1956) and Arnold Sommerfeld (1868–1951) were roughly contemporaneous . . . with one another, and also with Albert Einstein (1879–1955). While the contributions of the latter two to the early development of quantum mechanics are widely recognized, we tend to think of Whittaker as a *classical* physicist,[1] as a mathematician who drew his inspiration from predominantly classical applications,[2] and as an historian of physics concerned mainly with classical themes. But to his *The History of the Theories of Aether & Electricity*[3] he in 1953 added a Volume II which traced the history of quantum mechanics 1900–1926.[4]

[1] The first edition of his *Analytical Dynamics* appeared in 1904.

[2] His *Modern Analysis* appeared in 1902, when he was only 29 years old. It was revised and expanded with the assistance of G. N. Watson in 1915, and retains incidental quantum mechanical value as a mathematical resource.

[3] First published in 1910, revised in 1951.

[4] The volume is cited most often because in its Chapter II, writing under the title "The relativity theory of Poincaré and Lorentz," Whittaker seems to go unaccountably out of his way to speak dismissively of Einstein, who (Whittaker, on page 40, informs us) in 1905 "published a paper which set forth the relativity theory of Poincaré and Lorentz with some amplifications, which attracted much attention": see G. Holton, AJP **28**, 627 (1960); S. Goldberg, AJP **35**, 934 (1967); C. Cuvaj, AJP **36**, 1102 (1968); H. Schwartz, AJP **40**, 1272 (1972) for discussion of various aspects of this odd chapter in the history of the history of physics. Max Born, who at the time was also at the University of Edinburgh, reports in *The Born-Einstein Letters* (1971) that he had discussed the matter repeatedly and at length with "the old mathematician" who, however, remained adamant in his insistance that everything Einstein did had been done already by others (see Letter 102 at page 197). Whittaker's history of quantum mechanics was eclipsed by the Max Jammer's *The Conceptual Development of Quantum Mechanics* (1966) and, though it retains value, is seldom cited.

Near the end of that volume Whittaker departs from his self-imposed time frame to allude (at page 279) to some quantum mechanical work which he himself published in 1941. As it happens, I had come quite by accident upon the paper in question[5] in 1957, had recognized its relevance to my then on-going effort to understand earlier work by Dirac and subsequent work by Feynman and Schwinger, so had written an account of Whittaker's work into my research notes of the period. In the spring of 1968 I revisited the subject, and wrote the material which can be found on pages 68–83 in Chapter 3 of my QUANTUM MECHANICS (1967/68). Here I do much the same thing (if—I hope—from a somewhat deepened perspective) . . . for reasons which I now explain:

Whittaker sites only a solitary reference to the quantum literature (though in *Theories of Aether II* he tacitly acknowledges that he works within what Jammer,[4] in his §6.2, calls "the transformation theory," and in reaction to an impression conveyed by WKB theory) . . . and that is to the same brief Dirac paper[6] that inspired Feynman to cast quantum mechanics as an exercise in functional integration, Schwinger . . . as an exercise in functional differentiation.[7] Dirac/Feynman/Schwinger comprise a natural "package" in the conceptual development of quantum mechanics, and it is my thesis that Whittaker—though his work (which I have never seen cited) remains lost in obscurity—merits inclusion in that package. It contains, moreover, the seeds of some technical ideas which seem to me to be too valuable to be consigned to oblivion.

Preliminaries. With Whittaker, and in the interest only of notational simplicity, we look specifically/exclusively to the quantum mechanics of *one-dimensional time-independent* Hamiltonian systems $H(p,x)$, where x is understood to refer to an inertial Cartesian frame. We agree to put out of mind the problems which attend design of the quantization process

$$H(x,p) \longrightarrow \mathsf{H}, \text{ hermitian assembly of } \mathsf{x}\text{'s and } \mathsf{p}\text{'s}$$

Whittaker (like Schwinger) elects to work in the Heisenberg picture, where states $|\psi)$ are fixed/static/time-independent and the dynamical burden is born exclusively the hermitian operators representative of observables

$$\begin{aligned} \mathsf{A}_0 \rightarrow \mathsf{A}_t = \mathsf{U}^{-1}(t)\,\mathsf{A}_0\,\mathsf{U}(t) & \\ \mathsf{U}(t) \equiv e^{-\frac{i}{\hbar}\mathsf{H}\,t} \text{ is unitary} \end{aligned}$$

[5] "On Hamilton's principal function in quantum mechanics," Proc. Roy. Soc. (Edinburgh), Section A, **61**, 1 (1941).

[6] "The Lagrangian in quantum mechanics," Physikalische Zeitschrift der Sowjetunion, Band 3, Heft 1 (1933). The paper is reprinted in the "Schwinger Collection" *Selected Papers on Quantum Electrodynamics* (1958).

[7] See Jagdish Mehra & Kimball A. Milton, *Climbing the Mountain: The Scientific Biography of Julian Schwinger* (2000), pages 276, 315 and 612.

The spectrum of such an A_t is t-independent, but it drags its eigenbasis along on its back:

$$\mathsf{A}_t|a,t) = a|a,t) \quad \text{with} \quad \begin{cases} \int |a,t)\,da(a,t| = \mathsf{I} \\ \\ (a',t|a'',t) = \delta(a''-a') \end{cases}$$

From

$$|\psi) = \int |a,t)\,da\,\underbrace{(a,t|\psi)}_{t\text{-dependent } a\text{-components of } |\psi)}$$

we see that, though $|\psi)$ itself is immobile, its components (relative to the drifting A_t-basis) move:

$$(a',t'|\psi) = \int (a',t'|a'',t'')\,da''(a'',t''|\psi) \quad : \quad t' \geqslant t''$$

Here brought into prominence is the complex-number-valued object $(a',t'|a'',t'')$. This is the central object of the Schwinger formalism, a generalization of the propagator $(x,t|x_0,t_0)$ to which the Feynman formalism is addressed and which is the object studied by Whittaker.

Take A to be, in particular, the position operator x and adopt a simplified notation:

$$\mathsf{x}(t)|x,t) = x|x,t) \quad \text{will be written} \quad \begin{cases} \mathsf{X}|X) = X|X) & \text{at } t=0 \\ \mathsf{x}|\,x\,) = \,x\,|\,x\,) & \text{at generic } t>0 \end{cases}$$

Also, $\mathsf{p}(t)$ will be written P at $t=0$ and abbreviated p at generic $t>0$. Whittaker draws attention to the fact that while

$$\big[\mathsf{x}(t), \mathsf{p}(t)\big] = i\hbar\mathsf{I} \quad \text{holds at all times } t$$

nothing similarly simple can be said about the "mixed commutators"

$$\big[\mathsf{x},\mathsf{X}\big], \quad \big[\mathsf{x},\mathsf{P}\big], \quad \big[\mathsf{p},\mathsf{X}\big], \quad \big[\mathsf{p},\mathsf{P}\big]$$

—the values of which are system-dependent.

Whittaker makes critical/characteristic use of an instance of the "mixed representation trick," concerning which we now assemble some basic information. Trivially (by hermiticity)

$$(x\,|\,\mathsf{x}\,|X) = x\cdot(x\,|X) \quad \text{and} \quad (x\,|\mathsf{X}|X) = X\cdot(x\,|X)$$

while

$$
\begin{aligned}
(x|\mathsf{p}|X) &= \iint (x|\mathsf{p}|p)\,dp(p|y)\,dy(y|X)\\
&= \tfrac{1}{h}\iint p\,e^{\frac{i}{\hbar}(x-y)p}(y|X)\,dpdy\\
&= \tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\iint e^{\frac{i}{\hbar}(x-y)p}(y|X)\,\tfrac{dp}{h}dy\\
&= \tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\int \delta(x-y)(y|X)\,dy\\
&= +\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\,(x|X)\\
(x|\mathsf{P}|X) &= -\tfrac{\hbar}{i}\tfrac{\partial}{\partial X}(x|X) \quad \text{by a similar argument}
\end{aligned}
$$

Moreover, if F has been constructed by x,X-ordered substitution into $F(x,X)$

$$
\begin{aligned}
\mathsf{F} &= {}_{\mathsf{x}}\big[F(x,X)\big]_{\mathsf{X}}\\
&= \sum \text{terms of the ordered form } f(\mathsf{x})g(\mathsf{X})
\end{aligned}
$$

then

$$(x|\mathsf{F}|X) = F(x,X)\cdot(x|X)$$

Assume the existence of functions $p(x,X)$ and $P(x,X)$ such that

$$\mathsf{p} = {}_{\mathsf{x}}\big[p(x,X)\big]_{\mathsf{X}} \quad \text{and} \quad \mathsf{P} = {}_{\mathsf{x}}\big[P(x,X)\big]_{\mathsf{X}}$$

We are placed then in position to write

$$
\begin{aligned}
+\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\,(x|X) &= \ p(x,X)\cdot(x|X)\\
-\tfrac{\hbar}{i}\tfrac{\partial}{\partial X}(x|X) &= P(x,X)\cdot(x|X)
\end{aligned}
$$

Define a function $S(x,X)$ by

$$(x|X) \equiv e^{\frac{i}{\hbar}S(x,X)} \tag{1}$$

Then

$$
\left.
\begin{aligned}
p(x,X) &= +\frac{\partial S(x,X)}{\partial x}\\
P(x,X) &= -\frac{\partial S(x,X)}{\partial X}
\end{aligned}
\right\} \tag{2}
$$

which look as though they might have been lifted directly from *classical* mechanics (theory of canonical transformations/Hamilton-Jacobi theory).[8]

Notice finally that if we introduce

$$\mathsf{S} \equiv {}_{\mathsf{x}}\big[S(x,X)\big]_{\mathsf{X}} \tag{3}$$

[8] See equations (9–14a), (9–14b) and (10–7) in Herbert Goldstein, *Classical Mechanics* (1980).

and allow ourselves to write

$$\frac{\partial \mathsf{S}}{\partial \mathsf{x}} \equiv {}_{\mathsf{x}}\!\left[\frac{\partial S(x,X)}{\partial x}\right]_{\mathsf{X}} \quad \text{and} \quad \frac{\partial \mathsf{S}}{\partial \mathsf{X}} \equiv {}_{\mathsf{x}}\!\left[\frac{\partial S(x,X)}{\partial X}\right]_{\mathsf{X}} \tag{4}$$

then we have

$$\left.\begin{aligned} \mathsf{p} &= +\frac{\partial \mathsf{S}}{\partial \mathsf{x}} \\ \mathsf{P} &= -\frac{\partial \mathsf{S}}{\partial \mathsf{X}} \end{aligned}\right\} \tag{5}$$

since if we wrap $(x|$ and $|X)$ around (5) we recover (2). Equations (5) comprise what Whittaker, in his §3, calls "Dirac's theorem on $(x|X)$."

Whittaker's "quantum mechanical Hamilton-Jacobi equation." On pages 73–75 in Chapter 3 of QUANTUM MECHANICS (1967/68) I give a renotated variant of the rather clumsy argument to which Whittaker devotes his §4. On the day after I rehearsed that argument in class, Arthur Ogus—then my student, but for the last quarter century a professor of mathematics at UC/Berkeley—presented me with the alternative argument reproduced below, which is at once more transparent and more general.

Write

$$\mathsf{H} = {}_{\mathsf{x}}\big[\mathcal{H}(x,p)\big]_{\mathsf{p}} = {}_{\mathsf{x}}\big[h(x,X)\big]_{\mathsf{X}} \tag{6}$$

It is a corollary of the definition (1) that

$$\tfrac{\partial}{\partial t}(x|X) = \tfrac{i}{\hbar}\tfrac{\partial S(x,X)}{\partial t}\cdot(x|X)$$

On the other hand, we have (since the motion of eigenstates in the Heisenberg picture is retrograde relative to the motion of states in the Schrödinger picture) $|x) = e^{+\frac{i}{\hbar}\mathsf{H}t}|X)$ or $(x| = (X|e^{-\frac{i}{\hbar}\mathsf{H}t}$ giving $\frac{\partial}{\partial t}(x| = -\frac{i}{\hbar}(x|\mathsf{H}$ whence

$$\begin{aligned} &= -\tfrac{i}{\hbar}(x|\mathsf{H}|X) \\ &= -\tfrac{i}{\hbar}h(x,X)\cdot(x|X) \end{aligned}$$

from which follows this LEMMA:

$$h(x,X) + \tfrac{\partial S(x,X)}{\partial t} = 0 \tag{7}$$

We now have

$$\begin{aligned} (x|\tfrac{\partial \mathsf{S}}{\partial t}|p) &= \int (x|\tfrac{\partial \mathsf{S}}{\partial t}|X)\,dX\,(X|p) \\ &= \int \tfrac{\partial S(x,X)}{\partial t}(x|X)\,dX\,(X|p) \\ &= -\int h(x,X)(x|X)\,dX\,(X|p) \quad \text{by the LEMMA} \\ &= -\int (x|\mathsf{H}|X)\,dX\,(X|p) \\ &= -(x|\mathsf{H}|p) \end{aligned}$$

which, since valid for all $(x|$ and $|p)$, entails

$$\mathsf{H} = -\frac{\partial \mathsf{S}}{\partial t} \tag{8}$$

which joins (5) in its mimicry of an equation standard to classical mechanics. Drawing finally upon (6) and (5) we obtain

$$_{\mathsf{x}}\Big[\mathcal{H}(x,p)\Big]_{\mathsf{p}=\frac{\partial \mathsf{S}}{\partial \mathsf{x}}} + \frac{\partial \mathsf{S}}{\partial t} = \mathbf{0} \tag{9}$$

which states simply that the propagator satisfies the Schrödinger equation, but possesses the design of the classical Hamilton-Jacobi equation.

Schrödinger built on the observation that if S satisfies the H-J equation then $\psi \equiv e^{\frac{i}{\hbar}S}$ satisfies an equation that becomes linear—becomes the "Schrödinger equation"—upon abandonment of a term; inversely, if ψ satisfies the Schrödinger equation then $S \equiv \frac{\hbar}{i}\log\psi$ satisfies the Hamilton-Jacobi equation in leading WKB approximation. Whittaker, with those familiar facts in mind, stresses that the H-J equation carries over *exactly* into quantum mechanics <u>provided $H(x,p)$ and $S(x,t;X,0)$ are properly reinterpreted</u>. This observation requires some commentary:

The classical H-J equation

$$H\big(x, \tfrac{\partial S}{\partial x}\big) + \tfrac{\partial S}{\partial x} = 0$$

admits of infinitely *many solutions*, each of which serves to describe the $H(x,p)$-induced dynamical drive of a curve $p(x,t) = \frac{\partial}{\partial x}S(x,t)$ inscribed on phase space. A particular solution of special importance is

$$\begin{aligned} S(x,t;x_0,t_0) &= \int_{t_0}^{t} L(\text{dynamical path})\,dt \\ &= \text{2-point ``dynamical action'' function} \\ &= \text{Hamilton's ``principal function''} \\ &= \text{Legendre generator of } \big\{x,p\big\} \xleftarrow[t]{\quad} \big\{x_0,p_0\big\} \end{aligned}$$

which satisfies a *pair* of H-J equations (each the time-reverse of the other)

$$\begin{aligned} H\big(x,+\tfrac{\partial S}{\partial x}\big) + \tfrac{\partial S}{\partial t} &= 0 \\ H\big(x,-\tfrac{\partial S}{\partial x_0}\big) - \tfrac{\partial S}{\partial t_0} &= 0 \end{aligned}$$

—equations that jointly serve to describe the relationship between the Lie generator $H(x,p)$ and the Legendre generator $S(x,t;x_0,t_0)$ of the dynamical flow. It is with the classical 2-point theory that Whittaker has established formal quantum mechanical contact—"formal" because he interprets S to be the "quantum mechanical principal function" (defined at (1)) and finds that he must replace $H(x,p)$ by its "well-ordered" counterpart $\mathcal{H}(x,p)$ (defined at (6)). He ends up with a description of the relationship between H (which acts incrementally: $t \to t+\delta t$) and the (logarithm of the) propagator (which spans finite temporal intervals: $t_0 \to t$).

Classically, it follows from

$$S(x,t;x_0,t_0) = \int_{t_0}^{t} L\big(x(\tau),\dot{x}(\tau)\big)\,d\tau$$

that

$$\frac{dS}{dt} = L\big(x(t),\dot{x}(t)\big)\text{—displayed, however, as a function of } \big\{x,t;x_0,t_0\big\}$$

and L—thus displayed—is dynamically useless. Were we (with Whittaker) to write

$$\frac{d\mathsf{S}}{dt} = \mathsf{L} \quad : \quad \text{“Lagrangian operator”} \tag{10}$$

we would find ourselves in possession of a latently interesting object—but an object subject to that same criticism. The idea is most usefully pursued in the contexts provided by specific examples.

First illustrative application: harmonic oscillator & its free particle limit. Asim O. Barut, my undergraduate thesis advisor, once dampened my enthusiasm about some wild idea with these wise words: “How does your idea apply to the free particle, the oscillator, the Kepler problem? If it's unworkable/uninteresting in those cases it's not worth thinking about.” We look now to where Whittaker's train of thought leads in the instance

$$\begin{aligned} H(x,p) &= \tfrac{1}{2m}(p^2 + m^2\omega^2x^2) && : \quad \text{HARMONIC OSCILLATOR} \\ &\downarrow \\ &= \tfrac{1}{2m}p^2 \text{ in the limit } \omega\downarrow 0 && : \quad \text{FREE PARTICLE} \end{aligned}$$

In both cases we have

$$\mathsf{H} = {}_{\mathsf{x}}\big[H(x,p)\big]_{\mathsf{p}}$$

which is to say: the distinction between H and $\mathcal{H}$ is absent.

Whittaker follows initially in the footsteps of Schrödinger, writing

$$\begin{aligned} \mathsf{H} &= \hbar\omega\big(\mathsf{a}^+\mathsf{a} + \tfrac{1}{2}\mathsf{I}\big) \\ \mathsf{a} &\equiv \sqrt{m\omega/2\hbar}\,\big(\mathsf{x} + \tfrac{i}{m\omega}\,\mathsf{p}\big) \end{aligned}$$

The motion (in the Heisenberg picture) of the (non-hermitian) operator a is described

$$\dot{\mathsf{a}} = (i/\hbar)\big[\mathsf{H},\mathsf{a}\big] = i\omega\big[\mathsf{a}^+\mathsf{a},\mathsf{a}\big] = -i\omega\,\mathsf{a}$$

Therefore[9]

$$\begin{aligned} \mathsf{a} &= e^{-i\omega t}\,\mathsf{A} \\ \mathsf{a}^+ &= e^{+i\omega t}\,\mathsf{A}^+ \end{aligned}$$

[9] Here $\mathsf{a} \equiv \mathsf{a}(t)$ and $\mathsf{A} \equiv \mathsf{a}(0)$.

which when notated

$$\left.\begin{aligned}\mathsf{x} + \tfrac{i}{m\omega}\,\mathsf{p} &= e^{-i\omega t}\big(\mathsf{X} + \tfrac{i}{m\omega}\,\mathsf{P}\big)\\ \mathsf{x} - \tfrac{i}{m\omega}\,\mathsf{p} &= e^{+i\omega t}\big(\mathsf{X} - \tfrac{i}{m\omega}\,\mathsf{P}\big)\end{aligned}\right\}\tag{11}$$

leads quickly to the conclusion that

$$\left.\begin{aligned}\mathsf{p} &= +\frac{\partial\mathsf{S}}{\partial\mathsf{x}} = \tfrac{m\omega}{\sin\omega t}\big(\mathsf{x}\cos\omega t - \mathsf{X}\big)\\ \mathsf{P} &= -\frac{\partial\mathsf{S}}{\partial\mathsf{X}} = \tfrac{m\omega}{\sin\omega t}\big(\mathsf{x} - \mathsf{X}\cos\omega t\big)\end{aligned}\right\}\tag{12}$$

Evidently[10]

$$\mathsf{S} = \tfrac{m\,\omega}{2\sin\omega t}\Big\{\big(\mathsf{x}^2 + \mathsf{X}^2\big)\cos\omega t - 2\,\mathsf{x}\mathsf{X}\Big\} + \chi(t)\,\mathsf{I}$$

To evaluate $\chi(t)$ we—for the first time—draw upon the "quantum mechanical H-J equation" (9), which the present instance reads

$$\frac{\partial\mathsf{S}}{\partial t} = -\Big\{\frac{1}{2m}\Big(\frac{\partial\mathsf{S}}{\partial\mathsf{x}}\Big)^2 + \frac{1}{2}m\omega^2\,\mathsf{x}^2\Big\}$$

and after a little manipulation gives

$$\chi'(t)\,\mathsf{I} = \tfrac{m\,\omega^2}{2\sin^2\omega t}\big(\mathsf{X}\,\mathsf{x} - \mathsf{x}\,\mathsf{X}\big)\cos\omega t$$

But $\big[\mathsf{p},\mathsf{x}\big] = \big[\tfrac{m\omega}{\sin\omega t}\big(\mathsf{x}\cos\omega t - \mathsf{X}\big),\mathsf{x}\big] = -\tfrac{m\omega}{\sin\omega t}\big[\mathsf{X},\mathsf{x}\big] = (\hbar/i)\,\mathsf{I}$ so

$$\begin{gathered}= -\tfrac{\hbar}{2i}\omega\cot\omega t\\ \Downarrow\\ \chi(t) = -\tfrac{\hbar}{i}\log\sqrt{\sin\omega t} + \text{constant}\end{gathered}$$

We are in position now to write

$$(x,t|X,0) = e^{\frac{i}{\hbar}S(x,t;X,0)}$$

where the recently surpressed time-variables have been reinstated, and where according to (3)

$$\begin{aligned}S(x,t;X,0) &= \frac{(x|\mathsf{S}|X)}{(x,X)}\\ &= \tfrac{m\,\omega}{2\sin\omega t}\Big\{\big(x^2 + X^2\big)\cos\omega t - 2\,xX\Big\} - \tfrac{\hbar}{i}\log\sqrt{\sin\omega t} + \text{constant}\end{aligned}$$

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[10] Note the x,X-ordering:

$$\mathsf{S} = {}_{\mathsf{x}}\Big[\underbrace{\tfrac{m\omega}{2\sin\omega t}\Big\{\big(x^2 + X^2\big)\cos\omega t - 2\,xX\Big\} + \chi(t)}_{S(x,X)}\Big]_{\mathsf{X}}$$

Also that S is non-hermitian unless $\big[\mathsf{x},\mathsf{X}\big] = \mathbf{0}$ and $\chi(t)$ is real—neither of which turn out to be the case.

In short:

$$(x,t;X,0) = \lambda \cdot \frac{1}{\sqrt{\sin \omega t}} e^{\frac{i}{\hbar}\left\{\frac{m\omega}{2\sin \omega t}(x^2+X^2)\cos \omega t - 2xX\right\}} \tag{13.1}$$

To evaluate the multiplicative constant λ we can proceed either from the composition rule

$$(x|X) = \int (x|y)\, dy (y|X)$$

($i.e.$, from completeness, which becomes an exercise in Gaussian integration) or from the requirement that

$$\lim_{t\downarrow 0}(x|X) = \delta(x - X)$$

($i.e.$, from orthonormality, which becomes an exercise in δ-representation theory); either procedure supplies (I skip the familiar details)

$$\lambda = \sqrt{m\omega/ih} \tag{13.2}$$

On the other hand, we have the "spectral representation" of the propagator

$$(x,t;X,0) = \sum_{n=0}^{\infty} e^{-\frac{i}{\hbar}E_n t}\, \psi_n(x)\psi_n^*(X) \tag{14.1}$$

where in the present instance

$$\left.\begin{aligned} E_n &= \hbar\omega(n+\tfrac{1}{2}) \\ \psi_n(x) &= \left(\tfrac{2m\omega}{h}\right)^{\frac{1}{4}} \tfrac{1}{\sqrt{2^n n!}}\, e^{-\frac{1}{2}(m\omega/\hbar)x^2} H_n\left(\sqrt{\tfrac{m\omega}{\hbar}}\, x\right) \end{aligned}\right\} \tag{14.2}$$

In setting

$$\text{right side of (14)} = \text{right side of (13)}$$

Whittaker obtains what he calls "a quantum-mechanical deduction of Mehler's formula," the allusion being to a result first obtained by F. G. Mehler in 1866.[11] An identical result was achieved by Feynman in 1947 (and used by him to illustrate the power of the path-integral method), and by Schwinger (who in unpublished class notes used an elegant operator-ordering technique) a bit later, but neither seems to have been aware of the Mehler connection . . . or that Whittaker had been there first.[12]

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[11] See "Jacobi's theta transformation & Mehler's formula: their interrelation, and their role in the quantum theory of angular momentum" (2000).

[12] Whittaker, for his own part, appears to have been more interested in the mathematics than the physics, and neglects to mention (did not notice?) that the $\{$etc.$\}$ in (13.1) is precisely the *classical action* for an oscillator—a point of which Feynman, at least, was very well aware.

Look now to the ramifications of (10). We have

$$\mathsf{L} \equiv \frac{d\mathsf{S}}{dt} = \frac{\partial \mathsf{S}}{\partial t} + \tfrac{m\omega}{2\sin\omega t}\Big\{\cos\omega t\cdot\frac{d\mathsf{x}^2}{dt} - 2\frac{d\mathsf{x}}{dt}\mathsf{X}\Big\}$$

which by

$$\begin{aligned}\frac{d\mathsf{x}}{dt} &= -\tfrac{1}{i\hbar}\big[\mathsf{H},\mathsf{x}\big] = -\tfrac{1}{i\hbar}\big[\tfrac{1}{2m}\mathsf{p}^2,\mathsf{x}\big] = \tfrac{1}{m}\mathsf{p}\\ \frac{d\mathsf{x}^2}{dt} &= \mathsf{x}\frac{d\mathsf{x}}{dt} + \frac{d\mathsf{x}}{dt}\mathsf{x} = \tfrac{1}{m}\big(\mathsf{x}\,\mathsf{p} + \mathsf{p}\,\mathsf{x}\big) = \tfrac{1}{m}\big(2\mathsf{p}\,\mathsf{x} + i\hbar\mathsf{I}\big)\\ \frac{\partial\mathsf{S}}{\partial t} &= -\mathsf{H}\end{aligned}$$

leads, after a little straightforward algebra, to

$$\begin{aligned}\mathsf{L} &= \tfrac{1}{2m}\mathsf{p}^2 - \tfrac{1}{2}m\omega^2\mathsf{x}^2 + \underbrace{i\hbar\,\tfrac{\omega\cot\omega t}{2}\,\mathsf{I}}_{=\frac{d}{dt}\left(i\hbar\log\sqrt{\sin\omega t}\,\right)\ :\ \text{a gauge term}} \qquad (15)\\ &= \tfrac{1}{2}m\dot{\mathsf{x}}^2 - \tfrac{1}{2}m\omega^2\mathsf{x}^2 + (\text{gauge term})\end{aligned}$$

The L of (15) was obtained by Whittaker himself in his §7. Other descriptions of L are developed on page 80 of the old notes cited in the Introduction.

Notice that the imaginary gauge term contributes an imaginary additive term to $S(x,X)$, which accounts for the t-dependent amplitude factor (Feynman's "normalization factor," the dwelling place of the "Van Vleck determinant") in

$$(x,t;x_0,0) = (\text{amplitude})\cdot e^{i(\text{phase})}$$

and that its abandonment or adjustment would therefore do mischief.

A far less trivial example. Whittaker, broadly informed classical analyst that he was, was aware that Mehler's formula—fundamental to the theory of Hermite polynomials—is representative of a *class* of such formulae. And that within that class falls "Lebedeff's formula, fundamental to the theory of generalized Laguerre polynomials."[13] Intent upon constructing a "quantum-mechanical deduction of the Lebedeff formula," Whittaker plucks from unmotivated thin air the (dimensionally nonsensical) "Hamiltonian"

$$\begin{aligned}\mathsf{H} &= \mathsf{p}\,\mathsf{x}\,\mathsf{p} + \frac{A}{\mathsf{x}} + B\mathsf{x} \qquad (16)\\ &= {}_{\mathsf{x}}\big[\mathcal{H}(x,p)\big]_{\mathsf{p}} \quad \text{with} \quad \mathcal{H}(x,p) = \underbrace{xp^2 + \frac{A}{x} + Bx}_{H(x,p)} - i\hbar p\end{aligned}$$

[13] Wera Lebedeff, who worked with Hilbert, took a PhD from Göttingen in 1906. Lebedeff's formula appears for the first time in Mathematische Annalen **64**, 388 (1907). Whittaker remarks that the formula was rediscovered by Hille (Proc. Nat. Acad. Sci. **12**, 261, 265 & 348 (1926)), Hardy (Journ. Lond. Math. Soc. **7**, 138 & 192 (1932)) and many others.

The example acquires special interest from the circumstances that $H(x,p)$ does *not* depend (at most) quadratically upon its arguments and, moreover, the distinction between $\mathcal{H}(x,p)$ and $H(x,p)$ has become non-trivial (though it vanishes in the limit $\hbar \downarrow 0$).

Whittaker's motivation is entirely mathematical, and has only formally to do with quantum mechanics.[14] It is rooted in properties of the generalized Laguerre polynomials, which I now summarize.[15] We have this definition

$$L_n^a(z) \equiv \tfrac{1}{n!}[e^{-z}z^a]^{-1}\big(\tfrac{d}{dz}\big)^n\big\{[e^{-z}z^a]z^n\big\}$$

and an integral representation

$$= \tfrac{1}{n!}e^z z^{-\frac{1}{2}a}\int_0^\infty e^{-t}t^{n+\frac{1}{2}a}J_a(2\sqrt{zt})\,dt$$

that establishes contact with the theory of Bessel functions. The functions are orthogonal in this sense

$$\int_0^\infty L_m^a(z)L_n^a(z)\,e^{-z}z^a\,dz = \tfrac{\Gamma(n+a+1)}{n!}\delta_{mn}$$

so if we introduce[16]

$$\varphi_n(z) \equiv \Big[\tfrac{n!}{\Gamma(n+a+1)}e^{-z}z^a\Big]^{\frac{1}{2}}L_n^a(z) \tag{17}$$

we have

$$\int_0^\infty \varphi_m(z)\,\varphi_n(z)\,dz = \delta_{mn}$$

The functions $\Phi_n(z) \equiv e^{-\frac{1}{2}z}\varphi_n(z)$ are reported by Abramowitz & Stegun to satisfy $z\Phi_n'' + (z+1)\Phi_n' + (n + \frac{a}{2} + 1 - \frac{a^2}{4z})\Phi_n = 0$, so

$$z\varphi_n'' + \varphi_n' + \big\{-\tfrac{a^2}{4z} - \tfrac{1}{4}z + n + \tfrac{a+1}{2}\big\}\varphi_n = 0$$

which can be written

$$\Big\{\big(\tfrac{\hbar}{i}\tfrac{d}{dz}\big)z\big(\tfrac{\hbar}{i}\tfrac{d}{dz}\big) + \tfrac{\hbar^2a^2}{4z} + \tfrac{\hbar^2}{4}z\Big\}\varphi_n = \hbar^2\big(n + \tfrac{a+1}{2}\big)\varphi_n$$

The variable z is necessarily dimensionless. To achieve more immediate contact with the latent physics, write

$$z \equiv x/\ell \quad\text{and}\quad \psi_n(x) \equiv \tfrac{1}{\sqrt{\ell}}\varphi_n(x/\ell) \tag{18}$$

where x has the usual meaning, and ℓ is a "characteristic length." Multiplication

---

[14] He remarks that he has written "$\mathsf{p\,x\,p}$ rather than $\mathsf{x\,p}^2$ or $\mathsf{p}^2\mathsf{x}$ because [the former is hermitian while the latter two are not]" but that is a consideration rooted not so much in quantum mechanics as in classic Sturm-Lioville theory.

[15] I take as my source Chapter 22 in Abramowitz & Stegun.

[16] Here $n = 0, 1, 2, \ldots$ while the notationally surpressed index can assume any value $a > -1$.

of the preceding differential equation by $\frac{1}{2m\ell^2}$ then gives

$$\tfrac{1}{2m}\Big\{\tfrac{1}{\ell}\big(\tfrac{\hbar}{i}\tfrac{d}{dx}\big)x\big(\tfrac{\hbar}{i}\tfrac{d}{dx}\big)+\tfrac{\hbar^2a^2}{4\ell x}+\tfrac{\hbar^2}{4\ell^3}x\Big\}\psi_n=\tfrac{\hbar^2}{2m\ell^2}\big(n+\tfrac{a+1}{2}\big)\psi_n$$

which can be written

$$\mathsf{H}\psi_n=E_n\psi_n$$

where

$$\mathsf{H}\equiv\tfrac{1}{2m}\Big\{\tfrac{1}{\ell}\,\mathsf{p}\,\mathsf{x}\,\mathsf{p}+\frac{A}{\mathsf{x}}+B\mathsf{x}\Big\}\quad\text{with}\quad A=\tfrac{\hbar^2a^2}{4\ell}\text{ and }B=\tfrac{\hbar^2}{4\ell^3}$$

$$E_n=\tfrac{\hbar^2}{2m\ell^2}\big(n+\tfrac{a+1}{2}\big)\tag{19}$$

Whittaker has been content to set $2m=\ell=1$ and to make it appear that A and B are independently adjustable, though for his purposes they are in fact not: only the value of $a>-1$ is adjustable. Notice also that

$$=\hbar(\omega n+\omega_0)\quad\text{with}\quad\omega\equiv\tfrac{\hbar}{2m\ell^2}\text{ and }\omega_0=\tfrac{\hbar}{2m\ell^2}\tfrac{a+1}{2}$$

The spectrum is, in other words, "oscillator-like," but shifted. Writing

$$\begin{aligned}\mathsf{H}&=\tfrac{1}{2m\ell}\Big\{\mathsf{p}\,\mathsf{x}\,\mathsf{p}+\tfrac{\hbar^2a^2}{4\mathsf{x}}+\tfrac{\hbar^2}{4\ell^2}\mathsf{x}\Big\}\\&={}_{\mathsf{x}}\big[\mathcal{H}(x,p)\big]_{\mathsf{p}}\quad\text{with}\quad\mathcal{H}(x,p)=\underbrace{\tfrac{1}{2m\ell}\Big\{xp^2+\tfrac{\hbar^2a^2}{4x}+\tfrac{\hbar^2}{4\ell^2}x}_{H(x,p)}-i\hbar p\Big\}\end{aligned}\tag{20}$$

we are at first surprised to see the intrusion of $\hbar$'s into a "classical" Hamiltonian, but this is in fact a common feature of the "effective Hamiltonians" that arise when higher-dimensional systems are subjected to analysis by separation of variables.[17]

[17] For example: the 2-dimensional central force problem, in polar coordinates, reads

$$\Big\{-\tfrac{\hbar^2}{2m}\big[\tfrac{1}{r}\tfrac{\partial}{\partial r}r\tfrac{\partial}{\partial r}+\tfrac{1}{r^2}\tfrac{\partial^2}{\partial\theta^2}\big]+V(r)\Big\}\Psi=E\Psi$$

Set $\Psi(r,\theta)=\psi(r)e^{i\ell\theta}$ and obtain

$$\begin{aligned}\Big\{-\tfrac{\hbar^2}{2m}\big[\tfrac{1}{r}\tfrac{\partial}{\partial r}r\tfrac{\partial}{\partial r}\big]+V_{\text{eff}}(r)\Big\}\psi&=E\psi\\V_{\text{eff}}(r)&\equiv V(r)+\tfrac{\hbar^2\ell^2}{2mr^2}\end{aligned}$$

See page 12 in "Classical/quantum theory of 2-dimensional hydrogen" (1999) for the finer details.

We now have

$$
\begin{aligned}
(x,t;X,0) &= \sum_{n=0}^{\infty} e^{-i(\omega n+\omega_0)t}\psi_n(x)\psi_n(X)\\
&= \tfrac{1}{\ell}e^{-\theta_0}\sum_{n=0}^{\infty} e^{-i\theta n}\varphi_n(z)\varphi_n(Z) \quad \text{in dimensionless variables}
\end{aligned}
$$

(here $\theta \equiv \omega t$ is a "dimensionless time" variable, and $\theta_0 \equiv \omega_0 t$). "Lebedeff's formula" provides—in the tradition of Mehler—an alternative description of the spectral sum on the right.

I turn now to a renotated account of Whittaker's "quantum-mechanical deduction" of Lebedeff's formula, which he evidently considers to be the main contribution of his paper. His argument shows a high degree resourcefulness, and a willingness to undertake tediously detailed computational labor—qualities that are perhaps unexpected in a man at 67 (my own age, until last week).[18]

The Heisenberg equations of motion read

$$
\begin{aligned}
\dot{\mathsf{x}} &= \tfrac{1}{m\ell}\frac{\mathsf{x}\,\mathsf{p}+\mathsf{p}\,\mathsf{x}}{2}\\
\dot{\mathsf{p}} &= -\tfrac{1}{2m\ell}\mathsf{p}^2 - \tfrac{1}{2m}A\mathsf{x}^{-2} - \tfrac{1}{2m}B\,\mathsf{I}
\end{aligned}
$$

and (since nonlinear) appear to be relatively intractable. Whittaker skirts this problem by drawing upon what is already known about the eigenstates/values of H to construct matrix representations of x and (not of p but of) $\mathsf{x}\,\mathsf{p}$. From the known recurrence relation

$$
(n+1)L^a_{n+1}(z) = (2n+1+a-z)L^a_n(z) - (n+a)L^a_{n-1}(z)
$$

Whittaker extracts

$$
z\varphi_n = -\sqrt{n(n+a)}\,\varphi_{n-1} + (2n+1+a)\varphi_n - \sqrt{(n+1)(n+1+a)}\,\varphi_{n+1}
$$

which he uses (together with orthonormality) in

$$
\begin{aligned}
\mathbb{X} &= \|x_{mn}\|\\
x_{mn} &= e^{+i(m\theta+\theta_0)}(\psi_m, x\psi_n)e^{-i(n\theta+\theta_0)}\\
&= \ell(\varphi_m, z\varphi_n)e^{i(m-n)\theta}
\end{aligned}
$$

[18] We cannot know how substantial were the contributions of E. T. Copson, his colleague (and son-in-law) at St. Andrews, to whom he acknowledges his "indebtedness. . . for many helpful discussions while this investigation has been in progress." Of course, Whittaker benefited from knowing in advance the result he sought to establish.

to obtain

$$\mathbb{x} = \ell \begin{pmatrix} a+1 & -\xi_1 e^{-i\theta} & 0 & 0 & \cdots \\ -\xi_1 e^{+i\theta} & a+3 & -\xi_2 e^{-i\theta} & 0 & \cdots \\ 0 & -\xi_2 e^{+i\theta} & a+5 & -\xi_3 e^{-i\theta} & \cdots \\ 0 & 0 & -\xi_3 e^{+i\theta} & a+7 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

with $\xi_k \equiv \sqrt{k(k+a)}$. Similarly, from the known differential relation

$$z\tfrac{d}{dz}L_n^a(z) = nL_n^a(z) - (n+a)L_{n-1}^a(z)$$

he extracts

$$z\tfrac{d}{dz}\varphi_n = -\tfrac{1}{2}\sqrt{n(n+a)}\,\varphi_{n-1} - \tfrac{1}{2}\varphi_n + \tfrac{1}{2}\sqrt{(n+1)(n+1+a)}\,\varphi_{n+1}$$

giving $\mathbb{xp} = \|e^{im\theta}(\varphi_m, z\frac{\hbar}{i}\frac{d}{dz}\varphi_n)e^{-in\theta}\|$ whence

$$\mathbb{xp} = \tfrac{1}{2}\tfrac{\hbar}{i} \begin{pmatrix} -1 & -\xi_1 e^{-i\theta} & 0 & 0 & \cdots \\ +\xi_1 e^{+i\theta} & -1 & -\xi_2 e^{-i\theta} & 0 & \cdots \\ 0 & +\xi_2 e^{+i\theta} & -1 & -\xi_3 e^{-i\theta} & \cdots \\ 0 & 0 & +\xi_3 e^{+i\theta} & -1 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

Notice that we have only to set $\theta = 0$ to obtain descriptions of the "initial" matrices $\mathbb{X}$ and $\mathbb{XP} = \mathbb{PX} + i\hbar\,\mathbb{I}$. Whittaker at this point makes the clever observation that (because $e^{\pm i\theta} - 1 = \pm 2ie^{\pm\frac{1}{2}i\theta}\sin\frac{1}{2}\theta$)

$$\mathbb{x} - \mathbb{X} = 2i\ell\sin\tfrac{1}{2}\theta \cdot \begin{pmatrix} 0 & +\xi_1 e^{-i\frac{1}{2}\theta} & 0 & 0 & \cdots \\ -\xi_1 e^{+i\frac{1}{2}\theta} & 0 & +\xi_2 e^{-i\frac{1}{2}\theta} & 0 & \cdots \\ 0 & -\xi_2 e^{+i\frac{1}{2}\theta} & 0 & +\xi_3 e^{-i\frac{1}{2}\theta} & \cdots \\ 0 & 0 & -\xi_3 e^{+i\frac{1}{2}\theta} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

while $\mathbb{xp} + \mathbb{PX}$ is a scalar multiple of that *same matrix*:

$$\begin{aligned} \mathbb{xp} + \mathbb{PX} &= -\tfrac{\hbar}{i}\cos\tfrac{1}{2}\theta \cdot (\text{same matrix}) \\ &= \tfrac{\hbar}{2\ell}\cot\tfrac{1}{2}\theta \cdot (\mathbb{x} - \mathbb{X}) \end{aligned}$$

Whittaker arrives thus at this representation-independent implication of the equations of motion:

$$\mathsf{x}\,\mathsf{p} + \mathsf{X}\,\mathsf{P} = \tfrac{\hbar}{2\ell}\cot\tfrac{1}{2}\theta \cdot (\mathsf{x} - \mathsf{X})$$

Now another bit of cleverness: write

$$\mathsf{x}\big(\mathsf{p} - \tfrac{\hbar}{2\ell}\cot\tfrac{1}{2}\theta\,\mathsf{I}\big) = \big(-\mathsf{P} - \tfrac{\hbar}{2\ell}\cot\tfrac{1}{2}\theta\,\mathsf{I}\big)\mathsf{X} = \mathsf{W}$$

(W is a presently unknown operator, with the dimensions of action) and —drawing again upon (5)—conclude that

$$\begin{aligned}\mathsf{p} &= \tfrac{\hbar}{2\ell}\cot\tfrac{1}{2}\theta\,\mathsf{I} + \mathsf{x}^{-1}\mathsf{W} = \frac{\partial\mathsf{S}}{\partial\mathsf{x}}\\ -\mathsf{P} &= \tfrac{\hbar}{2\ell}\cot\tfrac{1}{2}\theta\,\mathsf{I} + \mathsf{W}\,\mathsf{X}^{-1} = \frac{\partial\mathsf{S}}{\partial\mathsf{X}}\end{aligned}$$

Evidently

$$\mathsf{S} = \tfrac{\hbar}{2\ell}\cot\tfrac{1}{2}\theta\cdot(\mathsf{x}+\mathsf{X}) + {}_{\mathsf{x}}\big[F(x,X)\big]_{\mathsf{X}}$$

and from $\mathsf{W} = \mathsf{x}\,{}_{\mathsf{x}}\big[\partial F/\partial x\big]_{\mathsf{X}} = {}_{\mathsf{x}}\big[\partial F/\partial X\big]_{\mathsf{X}}\mathsf{X}$ (*i.e.*, from $x\frac{\partial F}{\partial x} = X\frac{\partial F}{\partial X}$) we can conclude that $F(x,X)$ depends upon its arguments *only through their product*:

$$F(x,X) = f(xX)$$

To summarize our progress thus far: we have

$$\begin{aligned}K \equiv (x,t;X,0) &= \sum_{n=0}^{\infty} e^{-i(\omega n+\omega_0)t}\psi_n(x)\psi_n(X)\\ &= \tfrac{1}{\ell}e^{-\theta_0}\sum_{n=0}^{\infty} e^{-i\theta n}\varphi_n(z)\varphi_n(Z) \quad \text{in dimensionless variables}\\ &= e^{\frac{i}{\hbar}S}\end{aligned}$$

where S arises from (3) and has been discovered to have the form

$$\begin{aligned}S &= \tfrac{\hbar}{2\ell}\cot\tfrac{1}{2}\theta\cdot(x+X) + f(xX)\\ &= \tfrac{\hbar}{2}\cot\tfrac{1}{2}\theta\cdot(z+Z) + g(zZ) \quad \text{in dimensionless variables}\end{aligned}$$

At this point Whittaker is motivated by the distinctive design of Lebedeff's formula to depart from the advertised main line of his own theory: by-passing reference to the "quantum mechanical Hamilton-Jacobi equation," he works from the Schrödinger equation. Specifically, he observes that (because H and $e^{\frac{i}{\hbar}\mathsf{H}t}$ commute)

$$\Big\{z\tfrac{\partial^2}{\partial z^2} + \tfrac{\partial}{\partial z} - \tfrac{\alpha^2}{4z} - \tfrac{1}{4}z\Big\} \quad\text{and}\quad \Big\{Z\tfrac{\partial^2}{\partial Z^2} + \tfrac{\partial}{\partial Z} - \tfrac{\alpha^2}{4Z} - \tfrac{1}{4}Z\Big\}$$

achieve the same effect when applied to K. In other words,

$$\Big\{\Big(z\tfrac{\partial^2}{\partial z^2} - Z\tfrac{\partial^2}{\partial Z^2}\Big) + \Big(\tfrac{\partial}{\partial z} - \tfrac{\partial}{\partial Z}\Big) - \tfrac{\alpha^2}{4}\Big(\tfrac{1}{z} - \tfrac{1}{Z}\Big) + \tfrac{1}{4}\Big(Z - z\Big)\Big\}K = 0$$

But it has been found that z and Z enter into K only upon these combinations:

$$\begin{aligned}u &\equiv z + Z\\ v &= zZ\end{aligned}$$

Moreover,

$$\begin{aligned}
\left(\tfrac{1}{z}-\tfrac{1}{Z}\right) &= (Z-z)\cdot\tfrac{1}{v}\\
\left(\tfrac{\partial}{\partial z}-\tfrac{\partial}{\partial Z}\right) &= \left[\tfrac{\partial}{\partial u}+Z\tfrac{\partial}{\partial v}\right]-\left[\tfrac{\partial}{\partial u}+z\tfrac{\partial}{\partial v}\right]\\
&= (Z-z)\cdot\tfrac{\partial}{\partial v}\\
\left(z\tfrac{\partial^2}{\partial z^2}-Z\tfrac{\partial^2}{\partial Z^2}\right) &= z\left[\tfrac{\partial}{\partial u}+Z\tfrac{\partial}{\partial v}\right]^2-Z\left[\tfrac{\partial}{\partial u}+z\tfrac{\partial}{\partial v}\right]^2\\
&= \quad z\Big\{\tfrac{\partial^2}{\partial u^2}+2Z\tfrac{\partial^2}{\partial u\partial v}+\tfrac{\partial Z}{\partial u}\tfrac{\partial}{\partial v}+Z^2\tfrac{\partial^2}{\partial v^2}+Z\tfrac{\partial Z}{\partial v}\tfrac{\partial}{\partial v}\Big\}\\
&\quad -Z\Big\{\tfrac{\partial^2}{\partial u^2}+2z\tfrac{\partial^2}{\partial u\partial v}+\tfrac{\partial z}{\partial u}\tfrac{\partial}{\partial v}+z^2\tfrac{\partial^2}{\partial v^2}+z\tfrac{\partial z}{\partial v}\tfrac{\partial}{\partial v}\Big\}\\
&= (Z-z)\Big\{-\tfrac{\partial^2}{\partial u^2}+v\tfrac{\partial^2}{\partial v^2}\Big\}\\
&\qquad +\Big\{z\tfrac{\partial Z}{\partial u}+v\tfrac{\partial Z}{\partial v}-Z\tfrac{\partial z}{\partial u}-v\tfrac{\partial z}{\partial v}\Big\}\tfrac{\partial}{\partial v}
\end{aligned}$$

and from

$$\begin{pmatrix}\frac{\partial z}{\partial u} & \frac{\partial z}{\partial v}\\ \frac{\partial Z}{\partial u} & \frac{\partial Z}{\partial v}\end{pmatrix}=\begin{pmatrix}\frac{\partial u}{\partial z} & \frac{\partial u}{\partial Z}\\ \frac{\partial v}{\partial z} & \frac{\partial v}{\partial Z}\end{pmatrix}^{-1}=\begin{pmatrix}1 & 1\\ Z & z\end{pmatrix}^{-1}=\tfrac{1}{z-Z}\begin{pmatrix}z & -1\\ -Z & 1\end{pmatrix}$$

we learn that $\{\text{etc.}\}$ vanishes. The implication is that

$$(Z-z)\cdot\Big\{-\tfrac{\partial^2}{\partial u^2}+v\tfrac{\partial^2}{\partial v^2}+\tfrac{\partial}{\partial v}-\tfrac{\alpha^2}{4v}+\tfrac{1}{4}\Big\}K=0$$

But

$$K=e^{i\frac{u}{2}\cot\frac{1}{2}\theta}\cdot G(v)\quad\text{with}\quad G(v)\equiv e^{\frac{i}{\hbar}g(v)}$$

so

$$\Big\{v\tfrac{\partial^2}{\partial v^2}+\tfrac{\partial}{\partial v}-\tfrac{\alpha^2}{4v}+\tfrac{1}{4}(1+\cot^2\tfrac{1}{2}\theta)\Big\}G=0$$

Put $v=w^2$ and obtain

$$\tfrac{1}{4w^2}\Big\{w^2\tfrac{\partial^2}{\partial w^2}+w\tfrac{\partial}{\partial w}+w^2\csc^2\tfrac{1}{2}\theta-\alpha^2\Big\}G=0$$

Finally put $y=w\csc\frac{1}{2}\theta$ and obtain a standard form of Bessel's equation

$$\Big\{y^2\tfrac{d^2}{dy^2}+y\tfrac{d}{dy}+(y^2-\alpha^2)\Big\}G=0$$

The normalizable solutions are

$$G=\lambda\cdot J_\alpha(y)=\lambda\cdot J_\alpha\left(\frac{\sqrt{zZ}}{\sin\frac{1}{2}\theta}\right)$$

Whittaker is brought thus to the conclusion that

$$K=\lambda\cdot\exp\Big\{i\tfrac{z+Z}{2}\cot\tfrac{1}{2}\theta\Big\}\cdot J_\alpha\left(\frac{\sqrt{zZ}}{\sin\frac{1}{2}\theta}\right)\tag{21}$$

To fix the value of λ Whittaker appeals as before to the composition law (*i.e.*, to completeness), but the detailed argument is now more intricate. Write

$$(x,t;X,0) = \lambda\cdot\exp\Big\{i\tfrac{x+X}{2\ell}\cot\tfrac{1}{2}\theta\Big\}\cdot J_\alpha\bigg(\frac{\sqrt{xX}}{\ell\sin\frac{1}{2}\theta}\bigg) \tag{21.1}$$

Then

$$\begin{aligned}&\int(x,t_2;y,0)\,dy(y,t_1;X,0)\\ &\quad=\lambda_2\lambda_1\exp\Big\{i\tfrac{x}{2\ell}\cot\tfrac{1}{2}\theta_2\Big\}\exp\Big\{i\tfrac{X}{2\ell}\cot\tfrac{1}{2}\theta_1\Big\}\cdot\int_0^\infty e^{-p^2y}J_\alpha(\sqrt{y}\,a)J_\alpha(\sqrt{y}\,b)\,dy\end{aligned}$$

where

$$p^2\equiv -i\tfrac{1}{2\ell}\Big\{\cot\tfrac{1}{2}\theta_1+\cot\tfrac{1}{2}\theta_2\Big\},\quad a\equiv\frac{\sqrt{x}}{\ell\sin\frac{1}{2}\theta_2}\,,\quad b\equiv\frac{\sqrt{X}}{\ell\sin\frac{1}{2}\theta_1}$$

Write $y=t^2$ and obtain

$$\int_0^\infty e^{-p^2y}J_\alpha(\sqrt{y}\,a)J_\alpha(\sqrt{y}\,b)\,dy = 2\int_0^\infty e^{-p^2t^2}J_\alpha(ta)J_\alpha(tb)\,tdt$$

which by "Weber's second exponential integral"[19] becomes

$$=\tfrac{1}{p^2}\exp\Big\{-\tfrac{a^2+b^2}{4p^2}\Big\}I_\alpha\big(\tfrac{ab}{2p^2}\big)$$

But $\frac{ab}{2p^2}=i\frac{\sqrt{xX}}{\ell\sin\frac{1}{2}(\theta_1+\theta_2)}$ and[20] $I_\alpha(iy)=i^\alpha J_\alpha(y)$. Moreover $\frac{1}{p^2}=i2\ell\,\frac{\sin\frac{1}{2}\theta_1\sin\frac{1}{2}\theta_2}{\sin\frac{1}{2}(\theta_1+\theta_2)}$. So we have

$$\int(x,t_2;y,0)\,dy(y,t_1;X,0)=\lambda_2\lambda_1 2i\ell\,\frac{\sin\frac{1}{2}\theta_1\sin\frac{1}{2}\theta_2}{\sin\frac{1}{2}(\theta_1+\theta_2)}A_2A_1 i^\alpha J_\alpha\Big(\frac{\sqrt{xX}}{\ell\sin\frac{1}{2}(\theta_1+\theta_2)}\Big)$$

with

$$\begin{aligned}A_2&\equiv\exp\Big\{i\tfrac{x}{2\ell}\Big[\cot\tfrac{1}{2}\theta_2-\frac{\sin\frac{1}{2}\theta_1}{\sin\frac{1}{2}\theta_2\sin\frac{1}{2}(\theta_1+\theta_2)}\Big]\Big\}\\ &=\exp\Big\{i\tfrac{x}{2\ell}\cot\tfrac{1}{2}(\theta_1+\theta_2)\Big\}\\ A_1&=\exp\Big\{i\tfrac{X}{2\ell}\cot\tfrac{1}{2}(\theta_1+\theta_2)\Big\}\end{aligned}$$

---

[19] See I. S. Gradshteyn & I. M. Ryzhik, *Table of Integrals, Series & Products* (1965), where the identity in question—first obtained by H. Weber in 1868—appears as item **6.615**. G. N. Watson devotes §**13.31** in *Treatise on the Theory of Bessel Functions* (1966) to discussion of Weber's result, and reproduces a proof due to L. Gegenbauer (1876).

[20] See, for example, **50:11:3** in Spanier & Oldham's *Atlas of Functions*.

giving

$$\int (x,t_2;y,0)\,dy(y,t_1;X,0)$$
$$= \lambda_{12}\cdot\exp\Big\{i\tfrac{x+X}{2\ell}\cot\tfrac{1}{2}(\theta_1+\theta_2)\Big\}\cdot J_\alpha\left(\frac{\sqrt{xX}}{\ell\sin\frac{1}{2}(\theta_1+\theta_2)}\right)$$

with

$$\lambda_{12} = i^\alpha 2i\ell\,\tfrac{[\lambda_1\sin\frac{1}{2}\theta_1][\lambda_2\sin\frac{1}{2}\theta_2]}{\sin\frac{1}{2}(\theta_1+\theta_2)}$$

and are led by the evident pattern of this result to set

$$\lambda = \frac{i^{-\alpha}}{2i\ell\sin\frac{1}{2}\theta} \quad\text{with}\quad i^{-\alpha} = e^{-\frac{1}{2}i\pi\alpha} \tag{21.2}$$

where again θ is the "dimensionless time" parameter introduced several pages ago: $\theta \equiv \omega t = \frac{\hbar}{2m\ell^2}t$.

At (21) Whittaker has achieved his mathematical objective—"Lebedeff's formula"[20] —and with this accomplishment is content to abandon the subject. Though he exploited a quantum mechanically motivated train of thought he reveals no evident interest in the *physical* ramifications of his work.

Completeness of the Laguerre functions. We have now in hand the statement

$$\sum_{n=0}^\infty e^{-i(\omega n+\omega_0)t}\psi_n(x)\psi_n(X) \tag{22}$$
$$= \frac{e^{-\frac{1}{2}i\pi\alpha}}{2i\ell\sin\frac{1}{2}\theta}\exp\Big\{i\tfrac{x+X}{2\ell}\cot\tfrac{1}{2}\theta\Big\}\cdot J_\alpha\left(\frac{\sqrt{xX}}{\ell\sin\frac{1}{2}\theta}\right)$$

where

$$\psi_n(x) \equiv \tfrac{1}{\sqrt{\ell}}\varphi_n(x/\ell) \quad\text{with}\quad \varphi_n(z) \equiv \Big[\tfrac{n!}{\Gamma(n+a+1)}e^{-z}z^a\Big]^{\frac{1}{2}}L_n^a(z)$$

We look to the asymptotics (*i.e.*, to the limit $\theta\downarrow 0$) of the expression that stands on the right side of (22). The handbooks supply

$$J_\alpha(\xi) \sim \sqrt{\tfrac{2}{\pi\xi}}\cos\big(\xi - \tfrac{1}{2}\alpha\pi - \tfrac{1}{4}\pi\big) \quad\text{as}\quad \xi\to\infty$$

[20] In A. Erdélyi *et al*, *Higher Transcendental Functions II* (1953) the identity in question is presented in this more symmetric form

$$\sum_{n=0}^\infty \tfrac{n!}{\Gamma(n+\alpha+1)}L_n^\alpha(x)L_n^\alpha(y)z^n$$
$$= (1-z)^{-1}\exp\Big\{-z\tfrac{x+y}{1-z}\Big\}(xyz)^{-\frac{1}{2}\alpha}I_\alpha\Big(\tfrac{2\sqrt{xyz}}{1-z}\Big)$$

which the editors attribute to Hille-Hardy; they call the expression on the right a "bilinear generating function."

Therefore

$$
\begin{aligned}
\frac{e^{-\frac{1}{2}i\pi\alpha}}{2i\ell\sin\frac{1}{2}\theta}\exp\Big\{i\tfrac{x+X}{2\ell}\cot\tfrac{1}{2}\theta\Big\}\cdot J_\alpha\bigg(\frac{\sqrt{xX}}{\ell\sin\frac{1}{2}\theta}\bigg)&\\
\sim\frac{e^{-\frac{1}{2}i\pi\alpha}}{i\ell\theta}\exp\Big\{i\tfrac{x+X}{\ell\theta}\Big\}\cdot\tfrac{1}{2}\sqrt{\tfrac{\ell\theta}{\pi\sqrt{xX}}}\Big[&\exp\Big\{+i\big(\tfrac{2\sqrt{xX}}{\ell\theta}-\tfrac{1}{2}\alpha\pi-\tfrac{1}{4}\pi\big)\Big\}\\
&+\exp\Big\{-i\big(\tfrac{2\sqrt{xX}}{\ell\theta}-\tfrac{1}{2}\alpha\pi-\tfrac{1}{4}\pi\big)\Big\}\Big]\\
=\ \tfrac{1}{2}\sqrt{\tfrac{1}{\ell\theta\pi\sqrt{xX}}}\exp\Big\{-\tfrac{(\sqrt{x}+\sqrt{X})^2}{i\ell\theta}\Big\}&e^{i(-\frac{1}{2}\pi-\frac{1}{2}\pi\alpha-\frac{1}{2}\pi\alpha-\frac{1}{4}\pi)}\\
+\tfrac{1}{2}\sqrt{\tfrac{1}{\ell\theta\pi\sqrt{xX}}}\exp\Big\{-\tfrac{(\sqrt{x}-\sqrt{X})^2}{i\ell\theta}\Big\}&e^{i(-\frac{1}{2}\pi-\frac{1}{2}\pi\alpha+\frac{1}{2}\pi\alpha+\frac{1}{4}\pi)}\\
=\ \tfrac{1}{2}\big(\tfrac{1}{xX}\big)^{\frac{1}{4}}\sqrt{\tfrac{1}{i\ell\theta\pi}}\exp\Big\{-\tfrac{(\sqrt{x}+\sqrt{X})^2}{i\ell\theta}\Big\}&\cdot e^{i(-\frac{1}{2}\pi-\pi\alpha)}\\
+\tfrac{1}{2}\big(\tfrac{1}{xX}\big)^{\frac{1}{4}}\sqrt{\tfrac{1}{i\ell\theta\pi}}\exp\Big\{-\tfrac{(\sqrt{x}-\sqrt{X})^2}{i\ell\theta}\Big\}&
\end{aligned}
\tag{23}
$$

It is a familiar fact that

$$\delta(x-a)=\lim_{\varepsilon\downarrow 0}\tfrac{1}{\sqrt{\varepsilon\pi}}\exp\Big\{-\frac{(x-a)^2}{\varepsilon}\Big\}$$

so we appear to have

$$
\begin{aligned}
\tfrac{1}{2}\big(\tfrac{1}{xX}\big)^{\frac{1}{4}}\sqrt{\tfrac{1}{i\ell\theta\pi}}\exp\Big\{-\tfrac{(\sqrt{x}-\sqrt{X})^2}{i\ell\theta}\Big\}&=\tfrac{1}{2}\big(\tfrac{1}{xX}\big)^{\frac{1}{4}}\delta(\sqrt{x}-\sqrt{X}\,)\\
&=\tfrac{1}{2\sqrt{X}}\delta(\sqrt{x}-\sqrt{X}\,)
\end{aligned}
$$

It is familiar also[21] that if $g(x)$ possesses a solitary zero at X then

$$\delta\big(g(x)\big)=\frac{1}{|g'(X)|}\,\delta(x-X)$$

from which in the case $g(x)=\sqrt{x}-\sqrt{X}$ supplies

$$=\delta(x-X)\tag{24}$$

The Laguerre functions (17) live on the open interval $[0,\infty]$. Since $\sqrt{x}+\sqrt{X}$ does not vanish there, the leading term on the right side of (23) can be abandoned. We are left with

$$\sum_{n=0}^{\infty}\psi_n(x)\psi_n(X)=\delta(x-X)$$

which asserts the completeness of the function set $\big\{\psi_n(x)\big\}$. Mehler's formula can be used similarly (but much more easily) to establish the completeness of the Hermite functions (oscillator eigenfunctions), and—in the limit $\omega\downarrow 0$—to establish the completeness of the free particle eigenfunctions.

[21] See (13) in "Simplified production of Dirac δ-function identities" (1997).

The formulæ of Mehler and Lebedeff (also of Jacobi:[11] are there others?) owe their utility in this connection to the circumstance that each is of the form

$$\begin{aligned}\text{spectral sum, with } t \text{ “upstairs”} &= \begin{cases}\text{relatively complicated expression}\\ \text{with } t \text{ “downstairs”}\end{cases}\\ &\downarrow\\ &= \delta(x-X) \text{ in the limit } t\downarrow 0\end{aligned}$$

They acquire their physical interest from that same circumstance: they provide alternative descriptions of the quantum mechanical propagator. In Max Born's terminology, we encounter the

- “wave representation” on the left
- “particle representation” on the right

And has been emphasized successively by Dirac, Whittaker and Feynman, it is the latter that speaks most directly to the quantum-classical connection.

Classical physics of Whittaker's second example. The classical precursor of the class of quantum systems

$$\mathbf{H} = \tfrac{1}{2m\ell}\,\mathbf{p}\,\mathbf{x}\,\mathbf{p} + V(\mathbf{x})$$

is most naturally taken to be

$$H(x,p) = \tfrac{1}{2m\ell}\,xp^2 + V(x) \tag{25}$$

Elimination of p between

$$L = \dot{x}p - H(x,p)$$

and

$$\dot{x} = \tfrac{\partial}{\partial p}H(x,p) = \tfrac{1}{m\ell}\,xp$$

gives

$$L(x,\dot{x}) = \tfrac{1}{2}m\ell x^{-1}\dot{x}^2 - V(x) \tag{26}$$

The momentum conjugate to x is

$$p \equiv \tfrac{\partial}{\partial \dot{x}}L = m\ell x^{-1}\dot{x} = m\ell\,\tfrac{d}{dt}\log(x/\ell) \quad : \quad \text{necessarily } x > 0 \tag{27}$$

The equations of motion read

$$\tfrac{d}{dt}\big(m\ell x^{-1}\dot{x}\big) + \tfrac{1}{2}m\ell(x^{-1}\dot{x})^2 + V'(x) = 0 \tag{28.1}$$

which becomes

$$m\ell\big[\ddot{y} + \tfrac{1}{2}\dot{y}^2\big] + F(y) = 0 \tag{28.2}$$

with $y \equiv \log(x/\ell)$ and $F(y) \equiv V'(\ell e^y)$.

From the equation of motion it follows that we have “energy conservation” in the sense that the numerical value of the Hamiltonian is preserved:

$$E \equiv \tfrac{1}{2}m\ell x^{-1}\dot{x}^2 + V(x) \quad \text{is a constant of the motion}$$

Therefore

$$\dot{x} = \sqrt{\tfrac{2}{m\ell}x\big[E - V(x)\big]} \tag{29}$$

so the transit time ($X \to x$ with energy E) is given by

$$t(x, X; E) = \int_X^x \frac{1}{\sqrt{\frac{2}{m\ell} y\big[E - V(y)\big]}}\, dy$$

Whittaker's declared interest is in the cases $V(x) = \frac{1}{2m}(Ax^{-1} + Bx)$, and it is "to save some unnecessary writing" that (see again (19)) he sets $A = \frac{\hbar^2 a^2}{4\ell}$ and $B = \frac{\hbar^2}{4\ell^3}$. For such systems one has

$$\tfrac{2}{m\ell} x\big[E - V(x)\big] = \tfrac{2}{m}\big[-\tfrac{\hbar^2 a^2}{8m\ell^2} + E\cdot(x/\ell) - \tfrac{\hbar^2}{8m\ell^2}\cdot(x/\ell)^2\big]$$

Now Gradshteyn & Ryzhik, at **2.261** page 81, assign distinct values to the integral $\int(a + by + cy^2)^{-\frac{1}{2}}dy$, values determined by the signs of c and of $\Delta \equiv 4ac - b^2$. In the present application "c" is negative and

$$\Delta = \big(\tfrac{\hbar^2}{4m\ell^2}\big)^2 a^2 - E^2$$

which by (19) becomes

$$= \big(\tfrac{\hbar^2}{4m\ell^2}\big)^2\big[a^2 - (2n + a + 1)^2\big] < 0$$

We infer on this quantum mechanical evidence that the classically relevant statement is

$$\int^x \frac{1}{\sqrt{a + by + cy^2}}\, dy = -\frac{1}{\sqrt{-c}}\arcsin\frac{b + 2cx}{\sqrt{-\Delta}}$$

and on that basis obtain

$$\begin{aligned}\text{transit time } t &= -\sqrt{\tfrac{m\ell^2}{2}}\sqrt{\tfrac{8m\ell^2}{\hbar^2}}\arcsin\left(\frac{E - 2\frac{\hbar^2}{8m\ell^2}\xi}{\sqrt{E^2 - \big(\frac{\hbar^2}{4m\ell^2}\big)^2 a^2}}\right)\Bigg|_{\xi_0\equiv X/\ell}^{\xi\,\equiv\, x/\ell}\\ &= -\tfrac{2m\ell^2}{\hbar}\arcsin\left(\frac{\mathcal{E} - \xi}{\sqrt{\mathcal{E}^2 - a^2}}\right)\Bigg|_{\xi_0}^{\xi}\end{aligned}$$

where $\mathcal{E} \equiv \frac{4m\ell^2}{\hbar^2}E > a$ is a "dimensionless energy" parameter: $\xi \equiv x/\ell$ is "dimensionless length" and if we draw upon the notation $\omega \equiv \frac{\hbar}{2m\ell^2}$ introduced at (20) we have

$$\text{"dimensionless transit time" } \theta = \arcsin\left(\frac{\mathcal{E} - \xi}{\sqrt{\mathcal{E}^2 - a^2}}\right)\Bigg|_{\xi}^{\xi_0} \tag{30}$$

from which we learn that the motion of ξ is periodic. In dimensionless variables (29) reads

$$\tfrac{d\xi}{d\theta} = \sqrt{-a^2 + 2\mathcal{E}\xi - \xi^2} \tag{31}$$

which places turning points at

$$\xi_\pm = \mathcal{E} \pm \sqrt{\mathcal{E}^2 - a^2} \tag{32}$$

so we have

$$\begin{aligned}
\text{"dimensionless period"}\ \mathcal{T} &= 2\arcsin\left(\frac{\mathcal{E}-\xi}{\sqrt{\mathcal{E}^2-a^2}}\right)\Bigg|_{\xi_+}^{\xi_-}\\
&= 2\Big\{\arcsin(+1) - \arcsin(-1)\Big\} = \pi\\
\text{literal period}\ \tau = \pi/\omega &= \tfrac{4\pi m\ell^2}{\hbar}
\end{aligned} \tag{33}$$

and from the energy-independence of the period conclude that we are talking in a disguised way about a *harmonic* oscillator: Whittaker's second example is a disguised variant of his first example; Lebedeff's formula and Mehler's must be intimately related . . . as first became semi-evident when at (19) we obtained a spectrum that was "'oscillator-like,' but shifted."

In a first effort to penetrate the disguise we bring (see Abramowitz & Stegun: **4.4.32**)

$$\arcsin z_1 - \arcsin z_2 = \arcsin\left[z_1\sqrt{1-z_2^2} - z_2\sqrt{1-z_1^2}\,\right]$$

to the right side of (30), take the sine of both sides and (to avoid notational distractions) associate ξ_0 with the bisector $\frac{1}{2}(\xi_+ + \xi_-) = \mathcal{E}$ of the interval bounded by the turning points . . . to obtain

$$\begin{aligned}
\xi(\theta) &= \mathcal{E} + \sqrt{\mathcal{E}^2-a^2}\,\sin\theta \qquad (34.1)\\
&= (\text{mean value}) + (\text{amplitude})\sin\theta
\end{aligned}$$

Isoenergetic relaxation of the initial condition $\xi_0 = \mathcal{E}$ is accomplished by a simple phase adjustment: $\theta \mapsto \theta + \delta$. Figure 1 provides a direct geometrical interpretation of (34).

Working from (27) we are led to the

$$\begin{aligned}
\text{"dimensionless momentum"}\ \wp &\equiv \tfrac{\ell}{\hbar}p\\
&= \tfrac{m\ell^2}{\hbar}\xi^{-1}\dot{\xi}\\
&= \tfrac{1}{2}\xi^{-1}(d\xi/d\theta)
\end{aligned}$$

which by (34.1) entails

$$\wp(\theta) = \frac{1}{2}\frac{\sqrt{\mathcal{E}^2-a^2}\,\cos\theta}{\mathcal{E} + \sqrt{\mathcal{E}^2-a^2}\,\sin\theta} \tag{34.2}$$

Equations (34) give rise to the periodic phase flow contours shown in Figure 2.

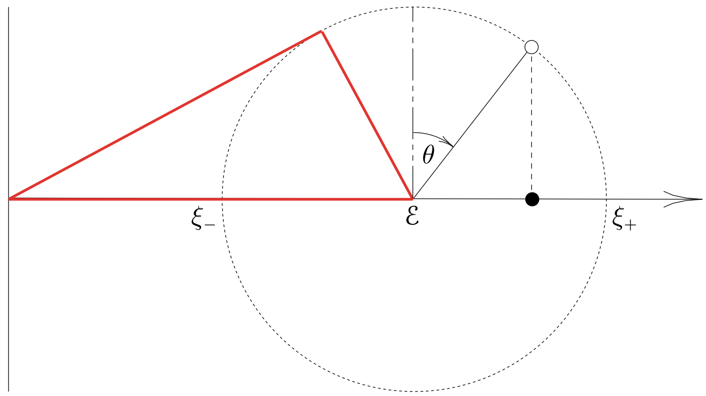

FIGURE 1: *"Displaced reference circle" that provides an elementary interpretation of (34). The circle*
- *is centered at* $\mathcal{E} = \frac{1}{2}(\xi_+ + \xi_-)$ *and*
- *has radius* $\sqrt{\mathcal{E}^2 - a^2} = \frac{1}{2}(\xi_+ - \xi_-)$, *so*
- *the tangent has length* a.

The representation point $\circ$ *proceeds uniformly around the circle, and completes a circuit in the* $\mathcal{E}$*-independent time* τ. *The parameter* a *is for Whittaker a system-parameterizing constant, while* $\mathcal{E} \geqslant a$ *is a dynamical constant of the motion.*

The phase area enclosed by such a contour is

$$\begin{aligned}\oint p\,dx &= \hbar \oint \wp\,d\xi \\ &= 2\hbar\int_{-\frac{1}{2}\pi}^{+\frac{1}{2}\pi} \wp(\theta)\xi'(\theta)\,d\theta \\ &= \hbar\int_{-\frac{1}{2}\pi}^{+\frac{1}{2}\pi} \frac{(\mathcal{E}^2 - a^2)\cos^2\theta}{\mathcal{E} + \sqrt{\mathcal{E}^2 - a^2}\sin\theta}\,d\theta\end{aligned}$$

Amazingly, the integral admits of elementary evaluation:

$$\begin{aligned}&= \hbar(\mathcal{E} - a)\pi \\ &= nh \quad \text{according to Planck/Bohr/Sommerfeld}\end{aligned}$$

Therefore $\mathcal{E} = 2n + a$, which in dimensioned physical variables becomes

$$E_n = \tfrac{\hbar^2}{2m\ell^2}(n + \tfrac{1}{2}a)$$

Semi-classical analysis has in this instance supplied an energy spectrum that agrees precisely with the exact spectrum (19) ...except in one anticipated detail: the zero-point term is absent.

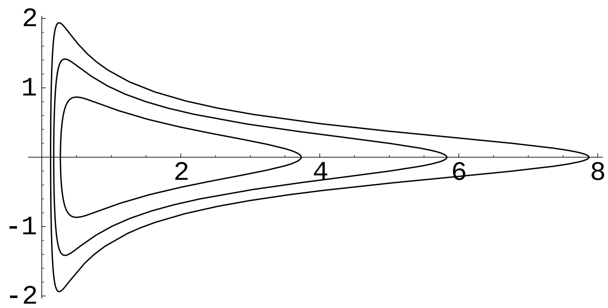

FIGURE 2: *Phase flow contours derived from (34). In preparing the figure I have set $a = 1$ and $\mathcal{E} = 2$ else 3 else 4. The ξ-axis runs $\rightarrow$, the $\wp$-axis runs $\uparrow$. The area enclosed by such contours was found on the preceding page to be remarkably easy to describe.*

To obtain a description of the dynamical trajectory that links (ξ_0, θ_0) to (ξ_1, θ_1) one might proceed this way: write

$$\xi_0 = \mathcal{E} + \sqrt{\mathcal{E}^2 - a^2}\big\{\sin\theta_0\cos\delta + \cos\theta_0\sin\delta\big\}$$
$$\xi_1 = \mathcal{E} + \sqrt{\mathcal{E}^2 - a^2}\big\{\sin\theta_1\cos\delta + \cos\theta_1\sin\delta\big\}$$

Solve for $\sin\delta$ and $\cos\delta$, to obtain equations of the form

$$\sin\delta = f(\xi_1, \theta_1; \xi_0, \theta_0; \mathcal{E})$$
$$\cos\delta = g(\xi_1, \theta_1; \xi_0, \theta_0; \mathcal{E})$$

From $f^2 + g^2 = 1$ obtain whence

$$\mathcal{E} = \mathcal{E}(\xi_1, \theta_1; \xi_0, \theta_0)$$

whence

$$\sin\delta = F(\xi_1, \theta_1; \xi_0, \theta_0)$$
$$\cos\delta = G(\xi_1, \theta_1; \xi_0, \theta_0)$$

Insert that data into $\xi = \mathcal{E} + \sqrt{\mathcal{E}^2 - a^2}\big\{\sin\theta\cos\delta + \cos\theta\sin\delta\big\}$ to obtain

$$\xi(\theta; \xi_1, \theta_1, \xi_0, \theta_0), \text{which gives back} \begin{cases} \xi_0 \text{ when } \theta = \theta_0 \\ \xi_1 \text{ when } \theta = \theta_1 \end{cases}$$

Mathematica encounters difficulty at none of those steps, but yields a final result which is too complicated to be informative. We can, however, hold those complications in suspension if (as is presently the case) our main objective is to describe the 2-point action function, which (see again (26)) by

$$\begin{aligned} L &= \tfrac{1}{2}m\ell^2(x/\ell)^{-1}(\dot{x}/\ell)^2 - \tfrac{1}{2m}\tfrac{\hbar^2}{4\ell^2}\big\{a^2(x/\ell)^{-1} + (x/\ell)\big\} \\ &= \tfrac{\hbar^2}{8m\ell^2}\Big[\xi^{-1}\big(\tfrac{d\xi}{d\theta}\big)^2 - (a^2\xi^{-1} + \xi)\Big] \end{aligned}$$

can be described

$$\begin{aligned} S[\text{dynamical path}] = \int L\,dt &= \tfrac{2m\ell^2}{\hbar}\int L\,d\theta \\ &= \hbar\int \tfrac{1}{4}\Big[\xi^{-1}\big(\tfrac{d\xi}{d\theta}\big)^2 - (a^2\xi^{-1} + \xi)\Big]\,d\theta \end{aligned} \tag{35}$$

It is in an effort to avoid bewildering complications, and to get a preliminary sense of the landscape . . . that I look now to the

$$\boxed{\text{CASE } a^2 = 0}$$

From

$$\begin{aligned} \xi_0 &= \mathcal{E}\big\{1 + \sin\theta_0\cos\delta + \cos\theta_0\sin\delta\big\} \\ \xi_1 &= \mathcal{E}\big\{1 + \sin\theta_1\cos\delta + \cos\theta_1\sin\delta\big\} \end{aligned}$$

we obtain

$$\begin{aligned} \sin\delta \equiv f(\xi_1,\theta_1;\xi_0,\theta_0;\mathcal{E}) &= \frac{(\mathcal{E}-\xi_1)\sin\theta_0 - (\mathcal{E}-\xi_0)\sin\theta_1}{\mathcal{E}\sin(\theta_1-\theta_0)} \\ \cos\delta \equiv g(\xi_1,\theta_1;\xi_0,\theta_0;\mathcal{E}) &= \frac{(\mathcal{E}-\xi_0)\sin\theta_1 - (\mathcal{E}-\xi_1)\sin\theta_0}{\mathcal{E}\sin(\theta_1-\theta_0)} \end{aligned}$$

whence

$$\mathcal{E}(\xi_1,\theta_1;\xi_0,\theta_0) = \frac{\xi_0 + \xi_1 \pm \sqrt{\xi_0\xi_1}(1+\cos[\theta_1-\theta_0])\sec\frac{1}{2}[\theta_1-\theta_0]}{2\sin^2\frac{1}{2}[\theta_1-\theta_0]}$$

The functions

$$\begin{aligned} F(\xi_1,\theta_1;\xi_0,\theta_0) &\equiv f(\xi_1,\theta_1;\xi_0,\theta_0;\mathcal{E}(\xi_1,\theta_1;\xi_0,\theta_0)) \\ G(\xi_1,\theta_1;\xi_0,\theta_0) &\equiv g(\xi_1,\theta_1;\xi_0,\theta_0;\mathcal{E}(\xi_1,\theta_1;\xi_0,\theta_0)) \end{aligned}$$

are a mess, and I must be content to let them reside in the mind of *Mathematica*, who supplies a result that can be written

$$\begin{aligned} \xi(\theta) &= \mathcal{E}(1 + G\sin\theta + F\cos\theta) \\ &= \frac{\xi_0\sin^2\frac{\theta-\theta_1}{2} - 2\sqrt{\xi_0\xi_1}\sin\frac{\theta-\theta_1}{2}\sin\frac{\theta-\theta_0}{2} + \xi_1\sin^2\frac{\theta-\theta_0}{2}}{\sin^2\frac{\theta_1-\theta_0}{2}} \\ &= \left(\frac{\sqrt{\xi_1}\sin\frac{\theta-\theta_0}{2} - \sqrt{\xi_0}\sin\frac{\theta-\theta_1}{2}}{\sin\frac{\theta_1-\theta_0}{2}}\right)^2 \end{aligned} \tag{36}$$

after much simplification. Note the elegant mechanism by which it comes about that $\xi(\theta_0)=\xi_0$, $\xi(\theta_1)=\xi_1$.

Working from (35: $a=0$) and (36) we compute

$$S=\hbar\underbrace{\Big\{\tfrac{1}{2}(\xi+\xi_0)\cot\tfrac{\theta-\theta_0}{2}-\sqrt{\xi_0\xi}\csc\tfrac{\theta-\theta_0}{2}\Big\}}_{\text{“dimensionless action” }\mathcal{S}(\xi,\theta;\xi_0,\theta_0)}\tag{37}$$

where I have now dropped the subscripts from ξ_1 and θ_1. Expansion in powers of $\theta-\theta_0$ yields a result

$$S=\hbar\Big\{\frac{\big(\sqrt{\xi}-\sqrt{\xi_0}\,\big)^2}{\theta-\theta_0}+\underbrace{\Big[\tfrac{1}{24}(\sqrt{\xi}-\sqrt{\xi_0}\,)^2-\tfrac{1}{8}(\xi+\xi_0)\Big]}_{=-\frac{1}{12}(x+\sqrt{xy}+y)}(\theta-\theta_0)+\cdots\Big\}\tag{38}$$

of latent relevance to the Feynman formalism.

From (25) we have (in the case $a=0$)

$$\begin{aligned}H&=\tfrac{1}{2m}\,(x/\ell)p^2+\tfrac{1}{2m}\tfrac{\hbar^2}{4\ell^2}(x/\ell)\\&=\tfrac{\hbar^2}{2m\ell^2}\underbrace{\Big\{\xi\wp^2+\tfrac{1}{4}\xi\Big\}}_{\text{“dimensionless Hamiltonian” }\mathcal{H}(\xi,\wp)}\end{aligned}\tag{39}$$

The Hamilton-Jacobi equation, in the present instance, reads

$$\tfrac{1}{2m}(x/\ell)\big(\tfrac{\partial S}{\partial x}\big)^2+\tfrac{1}{2m}\tfrac{\hbar^2}{4\ell^2}(x/\ell)+\tfrac{\partial S}{\partial t}=\tfrac{\hbar^2}{2m\ell^2}\Big\{\xi\big(\tfrac{\partial\mathcal{S}}{\partial\xi}\big)^2+\tfrac{1}{4}\xi+\tfrac{\partial\mathcal{S}}{\partial\theta}\Big\}=0$$

It is gratifying to be assured by *Mathematica* that if $\mathcal{S}$ is given by (37) then indeed

$$\left.\begin{aligned}\xi\;\big(\tfrac{\partial\mathcal{S}}{\partial\xi}\big)^2+\tfrac{1}{4}\xi\;+\tfrac{\partial\mathcal{S}}{\partial\theta}&=0\\\xi_0\big(\tfrac{\partial\mathcal{S}}{\partial\xi_0}\big)^2+\tfrac{1}{4}\xi_0-\tfrac{\partial\mathcal{S}}{\partial\theta_0}&=0\end{aligned}\right\}\tag{40}$$

Relatedly, it follows from (36) that the momentum at points along the path is given by

$$\wp(\theta)=\tfrac{1}{2}\xi^{-1}(d\xi/d\theta)=\tfrac{1}{2}\frac{(\sqrt{\xi}_1\cos\frac{\theta-\theta_0}{2}-\sqrt{\xi}_0\cos\frac{\theta-\theta_1}{2})}{(\sqrt{\xi}_1\sin\frac{\theta-\theta_0}{2}-\sqrt{\xi}_0\sin\frac{\theta-\theta_1}{2})}$$

The terminal momenta are given therefore by

$$\begin{aligned}\wp_1\equiv\wp(\theta_1)&=+\tfrac{1}{2}\Big\{\cot\tfrac{\theta_1-\theta_0}{2}-\sqrt{\xi_0/\xi_1}\csc\tfrac{\theta_1-\theta_0}{2}\Big\}\\\wp_0\equiv\wp(\theta_0)&=-\tfrac{1}{2}\Big\{\cot\tfrac{\theta_1-\theta_0}{2}-\sqrt{\xi_1/\xi_0}\csc\tfrac{\theta_1-\theta_0}{2}\Big\}\end{aligned}$$

which (as we verify) can be expressed

$$\wp_1=+\frac{\partial\mathcal{S}}{\partial\xi_1}\quad\text{and}\quad\wp_0=-\frac{\partial\mathcal{S}}{\partial\xi_0}\tag{41}$$

These results inspire confidence in the accuracy of (37).

The general *pattern* of the argument must persist in the

$$\boxed{\text{CASE } a^2 > 0}$$

but I must be content to reserve study of the daunting details for another occasion.

Transformational recovery of the classical harmonic oscillator. Let the equations

$$\xi = \eta^2 \quad \text{and} \quad \tfrac{1}{2}\theta = \vartheta$$

serve to introduce new dimensionless variables η and ϑ. By (37) we then have

$$\mathcal{S} = \frac{(\eta^2 + \eta_0^2)\cos(\vartheta - \vartheta_0) - 2\eta\eta_0}{2\sin(\vartheta - \vartheta_0)}$$

Write $y \equiv \ell\eta$ (physical dimensions of "length") and $\vartheta = \Omega t = \frac{1}{2}\omega t$ to obtain

$$S = \tfrac{\hbar}{m\ell^2\Omega}\cdot\left\{\frac{m\Omega}{2}\frac{(y^2 + y_0^2)\cos\Omega(t - t_0) - 2y\,y_0}{\sin\Omega(t - t_0)}\right\}$$

$$\tfrac{\hbar}{m\ell^2\Omega} = 2\tfrac{\hbar}{m\ell^2\omega} = 4$$

We recognize $\{\text{etc.}\}$ to be precisely the dynamical action of the simple oscillator

$$L = \tfrac{1}{2}m(\dot{y}^2 - \Omega^2 y^2)$$

Nor is this development surprising: we started from

$$L = \tfrac{1}{2}m\ell x^{-1}\dot{x}^2 - \tfrac{\hbar^2}{8m\ell^3}x$$

which by $x = y^2/\ell$ becomes

$$\begin{aligned} &= \tfrac{1}{2}my^{-2}(2y\dot{y})^2 - \tfrac{\hbar^2}{8m\ell^4}y^2 \\ &= 4\cdot\tfrac{1}{2}m\dot{y}^2 - 4\cdot\tfrac{1}{2}m\underbrace{\left(\tfrac{\hbar}{4m\ell^2}\right)^2}_{=\,(\frac{1}{2}\omega)^2\,=\,\Omega^2}y^2 \end{aligned}$$

The unsighly factors of 4 can be eliminated by $y \mapsto y \equiv 2y$.

The situation is, in fact, childishly simple: Suppose we wrote

$$\eta(t) = A\cos\Omega t$$

to describe the motion of an oscillator. We would then (by $\xi = \eta^2$) have

$$\xi(t) = A^2\cos^2\Omega t = \tfrac{1}{2}A^2(1 + \cos\omega t) \quad \text{with} \quad \omega = 2\Omega$$

The adjustment $\xi(t) \mapsto \eta(t)$ is illustrated in Figure 3.

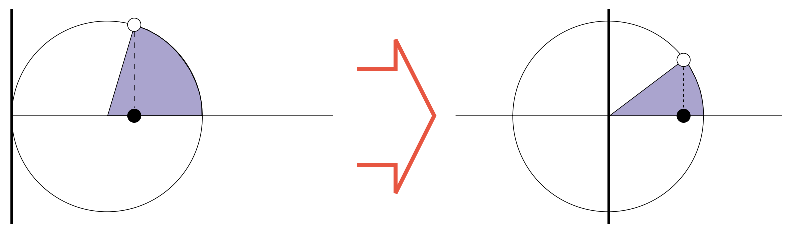

FIGURE 3: *The reference circle on the left lives in ξ-space. The transformation $\xi = \eta^2$ yields the figure on the right, which is the reference circle of a simple harmonic oscillator. Note that the rate of angular advance on the right is half that on the left ... for the simple reason that the point on the right passes through the origin twice per cycle.*

The preceding remarks are, I must emphasize, *special to the classical physics* and, within that context, *special to the case* $a^2 = 0$. Whittaker's two examples are—in at least that limited sense—coordinate transforms of one another. The question of immediate interest to me: Does that equivalence possess a quantum mechanical counterpart? To get a preliminary handle on the question we look to the canonical transform aspects of the classical theory.

The first of the following equations induces the second

$$\begin{aligned} q &\longmapsto Q = Q(q) \\ p &\longmapsto P = \tfrac{\partial q}{\partial Q} p \end{aligned} \tag{42}$$

The equations jointly entail Poisson bracket preservation

$$\big[Q, P\big] = \tfrac{\partial Q}{\partial q}\tfrac{\partial P}{\partial p} - \tfrac{\partial P}{\partial q}\tfrac{\partial Q}{\partial p} = \tfrac{\partial Q}{\partial q}\tfrac{\partial q}{\partial Q} - 0 = 1 = \big[q, p\big]$$

so describe a *canonical* transformation: canonical transformations of this specialized design are called "extended point transformations."[22] Look to the case $Q(q) \equiv q^2/\ell$: We have

$$\left.\begin{aligned} Q &= q^2/\ell \\ P &= \tfrac{\ell}{2q} p \end{aligned}\right\} \Longrightarrow \left\{\begin{aligned} q &= \sqrt{Q\ell} \\ p &= 2\sqrt{Q/\ell}\, P \end{aligned}\right.$$

Suppose $H(q,p) = \frac{1}{2m}(p^2 + m^2\omega^2 q^2)$. Then $\dot q = p/m$ and $\dot p = -m\omega^2 q$. Look to the effect of the canonical transformation:

$$H(q,p) \to K(Q,P) = 4 \cdot \tfrac{1}{2m\ell} Q\Big\{P^2 + m^2\big(\tfrac{1}{2}\omega\big)^2\ell^2\Big\} \tag{43}$$

[22] See E. T. Whittaker, *Analytical Dynamics* (4^{th} edition 1937), page 293.

The canonical equations of motion have assumed an unfamiliar appearance, but are readily seen to be equivalent to their (q, p)-counterparts. The point to notice is that the transformed Hamiltonian is (compare (20)) of the form

$$4 \cdot \tfrac{1}{2m}\Big\{\tfrac{1}{\ell}QP^2 + AQ^{-1} + BQ\Big\} \quad \text{with } A = 0$$

Can that latter restriction be relaxed? To the coordinate transformation let us conjoin a gauge transformation

$$L(q, \dot q) \quad\Longrightarrow\quad L\big(q(Q), \tfrac{\partial q(Q)}{\partial Q}\dot Q\big) + F(Q)\dot Q$$

In place of (42) we then have

$$\begin{aligned} q &\longmapsto Q = Q(q) \\ p &\longmapsto P = \tfrac{\partial q}{\partial Q}p + f(q) \\ &\qquad\qquad\qquad f(q) \equiv F(Q(q)) \end{aligned}$$

which is canonical by the same argument as before. Look to the case

$$\left.\begin{aligned} Q &= q^2/\ell \\ P &= \tfrac{\ell}{2q}p + f(q) \end{aligned}\right\} \Longrightarrow \left\{\begin{aligned} q &= \sqrt{Q\ell} \\ p &= 2\sqrt{Q/\ell}\,(P - F(Q)) \end{aligned}\right.$$

The transform of $H(q, p) = \frac{1}{2m}(p^2 + m^2\omega^2 q^2)$ has become

$$K(Q, P) = 4 \cdot \tfrac{1}{2m\ell}Q\Big\{\big(P - F\big)^2 + m^2\big(\tfrac{1}{2}\omega\big)^2\ell^2\Big\}$$

Let $F(Q) = \frac{1}{2}\hbar a Q^{-1}$. Then

$$\begin{aligned} &\downarrow \\ &= 4 \cdot \tfrac{1}{2m\ell}\Big\{QP^2 + \tfrac{1}{4}\hbar^2 a^2 Q^{-1} + \tfrac{1}{4}m^2\omega^2\ell^2 Q - \hbar a P\Big\} \end{aligned}$$

Recall that in oscillator theory one has a "natural length" $\ell \equiv \sqrt{\hbar/m\omega}$, and use $\omega^2 = \hbar^2/m^2\ell^4$ to obtain

$$= 4 \cdot \tfrac{1}{2m\ell}\Big\{QP^2 + \tfrac{\hbar^2 a^2}{4}Q^{-1} + \tfrac{\hbar^2 a^2}{4\ell^2}Q - \hbar a P\Big\} \tag{44}$$

This is very strongly reminiscent of Whittaker's (20), but I have thus far found no means for accomplishing the adjustment of the final term which would be required to make the agreement precise. Pending resolution of that problem, we must conclude that *only in the case* $a = 0$ is Whittaker's 2nd transformationally equivalent to a harmonic oscillator.

Recovery of Mehler's formula from Lebedeff's. Laguerre gave us an a-indexed *population* of orthogonal polynomials $L_n^a(x)$; Hermite a solitary set $H_n(x)$.[23] Reflecting this fact, there exists an a-indexed population of Lebedeff formulæ[24]

$$\sum_{n=0}^{\infty} e^{-i(n+\frac{a+1}{2})\theta}\tfrac{n!}{\Gamma(n+a+1)}e^{-\frac{1}{2}(X+Y)}(XY)^{\frac{a}{2}}L_n^a(X)L_n^a(Y) = \frac{e^{-\frac{1}{2}i\pi a}}{2i\sin\frac{1}{2}\theta}\exp\Big\{i\tfrac{X+Y}{2}\cot\tfrac{1}{2}\theta\Big\}\cdot J_a\bigg(\frac{\sqrt{XY}}{\sin\frac{1}{2}\theta}\bigg) \tag{45$_a$}$$

but only a solitary Mehler formula[25]

$$\sum_{k=0}^{\infty} e^{-i(k+\frac{1}{2})\vartheta}\tfrac{1}{\sqrt{\pi}\,2^k k!}e^{-\frac{1}{2}(x^2+y^2)}H_k(x)H_k(y) = \sqrt{\tfrac{1}{2\pi i\sin\vartheta}}\exp\Big\{i\tfrac{(x^2+y^2)\cos\vartheta-2xy}{2\sin\vartheta}\Big\} \tag{45}$$

In view of the central role played by Mehler's formula within the quantum theory of oscillators, and in the light of the discussion just concluded, it might appear natural to conjecture that $(44)_0 \Leftrightarrow (45)$. But how to turn J_0 into a complex exponential? The fact of the matter is such a conjecture is untenable, but that (45) can be obtained as a *linear combination* of $(44)_{+\frac{1}{2}}$ and $(44)_{-\frac{1}{2}}$!

The demonstration hinges on identities of three types. First we have[26]

$$\left.\begin{aligned} L_n^{-\frac{1}{2}}(x^2) &= \big(-\tfrac{1}{4}\big)^n\tfrac{1}{n!}H_{2n}(x)\\ L_n^{+\frac{1}{2}}(x^2) &= \tfrac{1}{2x}\big(-\tfrac{1}{4}\big)^n\tfrac{1}{n!}H_{2n+1}(x)\end{aligned}\right\} \tag{46}$$

which describes the Hermite polynomials in terms of certain associated Laguerre polynomials. Secondly, we need to know that the Bessel functions of fractional

---

[23] The *Mathematica* commands

```
Table[LaguerreL[n,a,x]],{n,0,4}]//TableForm
```

and

```
Table[HermiteH[n,x]],{n,0,4}]//TableForm
```

produce lists of examples.

[24] For the purposes of this (purely mathematical) discussion I have abandoned all physical parameters. To obtain $(40)_a$ use (17), (18) and (19) in (22) and set $\frac{\hbar}{2m\ell^2} = \ell = 1$. The formula thus obtained appears as (2.4/5) in Whittaker. The arguments have been capitalized for reasons that will soon become apparent.

[25] In (13) and (14) set $\frac{m\omega}{\hbar} = 1$ and write $\omega t \equiv \vartheta$. The formula thus obtained appears as (2.1/2) in Whittaker.

[26] See Spanier & Oldham, page 215. The identities given on page 84 of Magnus & Oberhettinger look different because phrased in terms of the so-called "alternative Hermite polynomials" $He_{2n}(x)$ and $He_{2n+1}(x)$.

order[27] are "elementary functions," and more specifically that

$$J_{+\frac{1}{2}}(x) = \sqrt{\tfrac{2}{\pi x}}\sin x \quad \text{and} \quad J_{-\frac{1}{2}}(x) = \sqrt{\tfrac{2}{\pi x}}\cos x \tag{47}$$

We will have need finally of these elemenary properties of the gamma function:[28]

$$n! = \Gamma(n+1) \tag{48.1}$$

$$\Gamma(z)\Gamma(z+\tfrac{1}{2}) = 4^z 2\sqrt{\pi}\,\Gamma(2z) \tag{48.2}$$

The identities (46) and (47) serve in themselves to indicate the pattern of the argument; we have only to cultivate the details:

Drawing first upon (470), we have

$$\text{right side of }(45)_{+\frac{1}{2}} = \frac{e^{-\frac{1}{4}i\pi}}{2i\sqrt{\sin\frac{1}{2}\theta}}\exp\Big\{i\tfrac{X+Y}{2}\cot\tfrac{1}{2}\theta\Big\}\cdot\sqrt{\tfrac{2}{\pi\sqrt{XY}}}\sin\left(\frac{\sqrt{XY}}{\sin\frac{1}{2}\theta}\right)$$

$$\text{right side of }(45)_{-\frac{1}{2}} = \frac{e^{+\frac{1}{4}i\pi}}{2i\sqrt{\sin\frac{1}{2}\theta}}\exp\Big\{i\tfrac{X+Y}{2}\cot\tfrac{1}{2}\theta\Big\}\cdot\sqrt{\tfrac{2}{\pi\sqrt{XY}}}\cos\left(\frac{\sqrt{XY}}{\sin\frac{1}{2}\theta}\right)$$

Notice that $e^{-\frac{1}{4}i\pi} = -ie^{+\frac{1}{4}i\pi}$. Addition therefore gives

$$\frac{e^{+\frac{1}{4}i\pi}}{2i\sqrt{\sin\frac{1}{2}\theta}}\sqrt{\tfrac{2}{\pi\sqrt{XY}}}\exp\Big\{i\tfrac{(X+Y)\cos\frac{1}{2}\theta-2\sqrt{XY}}{2\sin\frac{1}{2}\theta}\Big\}$$

which after some further simplification becomes

$$\left(\tfrac{1}{XY}\right)^{\frac{1}{4}}\cdot\sqrt{\tfrac{1}{2\pi i\sin\frac{1}{2}\theta}}\exp\Big\{i\tfrac{(X+Y)\cos\frac{1}{2}\theta-2\sqrt{XY}}{2\sin\frac{1}{2}\theta}\Big\} \tag{49}$$

This expression, according to Lebedeff, can also be described

$$\sum_{n=0}^\infty e^{-i(n+\frac{1}{2}+\frac{1}{4})\theta}\tfrac{n!}{\Gamma(n+\frac{1}{2}+1)}e^{-\frac{1}{2}(X+Y)}(XY)^{+\frac{1}{4}}L_n^{+\frac{1}{2}}(X)L_n^{+\frac{1}{2}}(Y)$$
$$+\sum_{n=0}^\infty e^{-i(n+\frac{1}{2}-\frac{1}{4})\theta}\tfrac{n!}{\Gamma(n-\frac{1}{2}+1)}e^{-\frac{1}{2}(X+Y)}(XY)^{-\frac{1}{4}}L_n^{-\frac{1}{2}}(X)L_n^{-\frac{1}{2}}(Y)$$

Change variables $X = x^2$, $Y = y^2$ and obtain

$$\sum_{n=0}^\infty e^{-i(n+\frac{1}{2}+\frac{1}{4})\theta}\tfrac{n!}{\Gamma(n+\frac{1}{2}+1)}e^{-\frac{1}{2}(x^2+y^2)}(xy)^{+\frac{1}{2}}L_n^{+\frac{1}{2}}(x^2)L_n^{+\frac{1}{2}}(y^2)$$
$$+\sum_{n=0}^\infty e^{-i(n+\frac{1}{2}-\frac{1}{4})\theta}\tfrac{n!}{\Gamma(n-\frac{1}{2}+1)}e^{-\frac{1}{2}(x^2+y^2)}(xy)^{-\frac{1}{2}}L_n^{-\frac{1}{2}}(x^2)L_n^{-\frac{1}{2}}(y^2)$$

Drawing now upon (46), the preceding expression becomes

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[27] See Magnus & Oberhettinger, page 18, or Spernier & Oldham, page 306. The functions $j_n(z) \equiv J_{n+\frac{1}{2}}(z)$ are called "spherical Bessel functions," and described under that head in most handbooks.

[28] See Magnus & Oberhettinger, page 1; Spanier & Oldham, page 414.

$$\begin{aligned}&\sum_{n=0}^{\infty} e^{-i(n+\frac{1}{2}+\frac{1}{4})\theta}\tfrac{1}{n!\Gamma(n+\frac{1}{2}+1)}e^{-\frac{1}{2}(x^2+y^2)}(xy)^{+\frac{1}{2}}\tfrac{1}{4xy}\big(\tfrac{1}{4}\big)^{2n}H_{2n+1}(x)H_{2n+1}(y)\\ &+\sum_{n=0}^{\infty} e^{-i(n+\frac{1}{2}-\frac{1}{4})\theta}\tfrac{1}{n!\Gamma(n-\frac{1}{2}+1)}e^{-\frac{1}{2}(x^2+y^2)}(xy)^{-\frac{1}{2}}\big(\tfrac{1}{4}\big)^{2n}H_{2n}(x)H_{2n}(y)\end{aligned}$$

which after some simplifying rearrangement reads

$$\begin{aligned}&\sum_{n=0}^{\infty} e^{-i(2n+1+\frac{1}{2})\frac{1}{2}\theta}\tfrac{1}{n!\Gamma(n+\frac{1}{2}+1)}e^{-\frac{1}{2}(x^2+y^2)}(xy)^{-\frac{1}{2}}\big(\tfrac{1}{4}\big)^{2n+1}H_{2n+1}(x)H_{2n+1}(y)\\ &+\sum_{n=0}^{\infty} e^{-i(2n+\frac{1}{2})\frac{1}{2}\theta}\tfrac{1}{n!\Gamma(n-\frac{1}{2}+1)}e^{-\frac{1}{2}(x^2+y^2)}(xy)^{-\frac{1}{2}}\big(\tfrac{1}{4}\big)^{2n}H_{2n}(x)H_{2n}(y)\end{aligned}$$

The identities (48) supply

$$\begin{aligned}n!\Gamma(n+\tfrac{1}{2}+1) &= \Gamma(n+1)\Gamma(n+1+\tfrac{1}{2})\\ &= 4^{-(n+1)}2\sqrt{\pi}\,\Gamma(2n+1+1)\\ &= 4^{-(n+1)}2\sqrt{\pi}\,(2n+1)!\\ n!\Gamma(n-\tfrac{1}{2}+1) &= \Gamma(n+\tfrac{1}{2})\Gamma(n+\tfrac{1}{2}+\tfrac{1}{2})\\ &= 4^{-(n+\frac{1}{2})}2\sqrt{\pi}\,\Gamma(2n+1)\\ &= 4^{-(n+\frac{1}{2})}2\sqrt{\pi}\,(2n)!\end{aligned}$$

so the preceding expression becomes

$$\begin{aligned}&\sum_{n=0}^{\infty} e^{-i(2n+1+\frac{1}{2})\frac{1}{2}\theta}\tfrac{1}{\sqrt{\pi}(2n+1)!}\big(\tfrac{1}{2}\big)^{2n+1}e^{-\frac{1}{2}(x^2+y^2)}(xy)^{-\frac{1}{2}}H_{2n+1}(x)H_{2n+1}(y)\\ &+\sum_{n=0}^{\infty} e^{-i(2n+\frac{1}{2})\frac{1}{2}\theta}\tfrac{1}{\sqrt{\pi}(2n)!}\big(\tfrac{1}{2}\big)^{2n}e^{-\frac{1}{2}(x^2+y^2)}(xy)^{-\frac{1}{2}}H_{2n}(x)H_{2n}(y)\\ &\qquad= (xy)^{-\frac{1}{2}}\cdot\sum_{k=0}^{\infty} e^{-i(k+\frac{1}{2})\frac{1}{2}\theta}\tfrac{1}{\sqrt{\pi}\,2^k k!}e^{-\frac{1}{2}(x^2+y^2)}H_k(x)H_k(y) \qquad (50.1)\\ &\qquad= \text{sum of left sides of }(45)_{\pm\frac{1}{2}}\end{aligned}$$

But at (49) we obtain a result which in present notation reads

$$\begin{aligned}&\text{sum of right sides of }(45)_{\pm\frac{1}{2}}\\ &\quad= (xy)^{-\frac{1}{2}}\cdot\sqrt{\tfrac{1}{2\pi i\sin\frac{1}{2}\theta}}\exp\Big\{i\tfrac{(x^2+y^2)\cos\frac{1}{2}\theta-2xy}{2\sin\frac{1}{2}\theta}\Big\} \qquad (50.2)\end{aligned}$$

At (50) we have recovered Mehler's formula (45). The intrusion of the (discardable) factor $(xy)^{-\frac{1}{2}}$ can be understood this way: If the coordinate transform properties of quantum theory are to contain the statement

$$\int |\Psi(X)|^2\,dX = \int |\psi(x)|^2\,dx$$

then the wave function must[29] transform as a *scalar density of weight* $\frac{1}{2}$:

$$X \to x \quad \text{induces} \quad \Psi(X) \to \psi(x) = \left|\tfrac{\partial X}{\partial x}\right|^{\frac{1}{2}} \Psi(X(x))$$

The transform of

$$\Psi_t(X) = \int G(X,Y;t)\Psi_0(Y)\,dY$$

then becomes

$$\psi_t(x) = \int g(x,y;t)\,\psi_0(y)\,dy$$

$$g(x,y;t) = \left|\tfrac{\partial X}{\partial x}\right|^{\frac{1}{2}} G(X(x),Y(y);t)\left|\tfrac{\partial Y}{\partial y}\right|^{\frac{1}{2}}$$

In the case of interest we have

$$= 2(xy)^{\frac{1}{2}} \cdot G(x^2,y^2;t)$$

When the factor is brought into play the former $(xy)^{-\frac{1}{2}}$ is killed, and the dangling 2 reflects the fact that Lebedeff's formula involves functions that are orthonormal on half the range of those contemplated by Mehler. To bring (45) and (50) into *precise* agreement we must set $\vartheta = \frac{1}{2}\theta$.

What quantum mechanical lessons can be extracted from the preceding discussion? Look back again to page 12, where we wrote equations that in a more detailed notation read

$$\begin{aligned} \tfrac{1}{2m}\Big\{\tfrac{1}{\ell}\big(\tfrac{\hbar}{i}\tfrac{d}{dx}\big)x\big(\tfrac{\hbar}{i}\tfrac{d}{dx}\big) + \tfrac{\hbar^2a^2}{4\ell x} + \tfrac{\hbar^2}{4\ell^3}x\Big\}\psi_{n,a} &= E_{n,a}\psi_{n,a} \\ E_{n,a} &= \tfrac{\hbar^2}{2m\ell^2}\big(n + \tfrac{a+1}{2}\big) \end{aligned}$$

with $\psi_{n,a}(x) = \frac{1}{\sqrt{\ell}}\Big[\frac{n!}{\Gamma(n+a+1)}e^{-x/\ell}(x/\ell)^a\Big]^{\frac{1}{2}}L_n^a(x/\ell)$. Notice that the parameter a enters squared into the design of the differential operator (Hamiltonian), but linearly into the description of its eigenvalues. We might be tempted to conclude that the spectrum has (except when $a = 0$) *two branches*, but such a conclusion is untenable: the functions $\{\psi_{n,+a}(x)\}$ are orthonormal and complete; so are the functions $\{\psi_{n,-a}(x)\}$ ...but the same cannot be said of the *union* of the two sets. In this respect Whittaker has misled us: he/we should have written

$$\begin{aligned} \underbrace{\tfrac{1}{2m}\Big\{\tfrac{1}{\ell}\big(\tfrac{\hbar}{i}\tfrac{d}{dx}\big)x\big(\tfrac{\hbar}{i}\tfrac{d}{dx}\big) + \tfrac{\hbar^2a^2}{4\ell x} + \tfrac{\hbar^2}{4\ell^3}x - \tfrac{\hbar^2 a}{2\ell^2}\Big\}}_{\mathsf{H}_a}\psi_{n,a} &= E_{n,a}\psi_{n,a} \\ E_{n,a} &= \tfrac{\hbar^2}{2m\ell^2}\big(n + \tfrac{1}{2}\big) \end{aligned} \tag{51}$$

[29] I discard this more general possibility:

$$\Psi(X) \to \psi(x) = e^{i\alpha(x)} \cdot \left|\tfrac{\partial X}{\partial x}\right|^{\frac{1}{2}} \Psi(X(x))$$

The Hamiltonians $\mathsf{H}_{\pm a}$ then refer to distinct physical systems, and we are deprived of any reason to conflate their spectra. Moreover,

$$E_{n,a} = \tfrac{\hbar^2}{2m\ell^2}\big(n+\tfrac{1}{2}\big) \quad\longrightarrow\quad \hbar\omega(n+\tfrac{1}{2}) \quad \text{if we set } \ell = \sqrt{\tfrac{2m\omega}{\hbar}}$$

The eigenvalues have become a-independent: *each* of the distinct systems H_a is *spectrally identical to a harmonic oscillator*.[30]

Taking H_a to be defined by (51), we have

$$\begin{aligned}
\tfrac{\partial}{\partial t}|\psi|^2 &= \tfrac{1}{i\hbar}\Big\{\psi^*\Big[\tfrac{1}{2m\ell}\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\big)x\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\big)\psi\Big] - \psi\Big[\tfrac{1}{2m\ell}\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\big)x\big(\tfrac{\hbar}{i}\tfrac{\partial}{\partial x}\big)\psi^*\Big]\Big\}\\
&= i\tfrac{\hbar}{2m\ell}\Big\{\psi^*\big(\tfrac{\partial}{\partial x}\big)x\big(\tfrac{\partial}{\partial x}\big)\psi - \psi\big(\tfrac{\partial}{\partial x}\big)x\big(\tfrac{\partial}{\partial x}\big)\psi^*\Big\}\\
&= i\tfrac{\hbar}{2m\ell}\Big\{\big(\tfrac{\partial}{\partial x}\big)\psi^* x\big(\tfrac{\partial}{\partial x}\big)\psi - \psi_x^* x\,\psi_x - \big(\tfrac{\partial}{\partial x}\big)\psi\, x\big(\tfrac{\partial}{\partial x}\big)\psi^* + \psi_x x\,\psi_x^*\Big\}\\
&= -\tfrac{\partial}{\partial x}\Big\{i\tfrac{\hbar}{2m\ell}\big[\psi\, x\,\psi_x^* - \psi^* x\,\psi_x\big]\Big\}
\end{aligned}$$

according to which *probability current* should in this context be defined

$$J(x,t) \equiv i\tfrac{\hbar}{2m\ell}\big[\psi\, x\,\psi_x^* - \psi^* x\,\psi_x\big]$$

If x is allowed to range on $(0,\infty)$ then we must require it to be the case for all

$$\psi_a(x) = \sum_{k=0}^{\infty} c_k\psi_{k,a}(x)$$

that $J(0,t) = J(\infty,t) = 0$ (all t). Which bring me to the point of this seeming digression: The normalized wave functions $\psi_{n,a}(x)$ behave unexceptionably (see Figures 4 & 5) as $x\to\infty$, but near the origin display (at least in the cases $a=-\frac{1}{2}$ and $a=0$) properties that we might naively dismiss as "unacceptable." We notice, however, that

$$J(x,t) = \sum_{j,k}(\text{function of } t)\cdot\big[\psi_{j,a}x\partial_x\psi_{k,a} - \psi_{k,a}x\partial_x\psi_{j,a}\big]$$

Mathematica reports that as we approach the origin

[30] Had Whittaker himself adopted such a viewpoint he would have been to this trivial *variant* of Lebedeff's $(45)_a$:

$$\sum_{n=0}^{\infty} e^{-i(n+\frac{1}{2})\theta}\tfrac{n!}{\Gamma(n+a+1)}e^{-\frac{1}{2}(X+Y)}(XY)^{\frac{a}{2}}L_n^a(X)L_n^a(Y) \qquad (45)_a$$

$$= e^{i\frac{1}{2}a\theta}\cdot\frac{e^{-\frac{1}{2}i\pi a}}{2i\sin\frac{1}{2}\theta}\exp\Big\{i\tfrac{X+Y}{2}\cot\tfrac{1}{2}\theta\Big\}\cdot J_a\bigg(\frac{\sqrt{XY}}{\sin\frac{1}{2}\theta}\bigg)$$

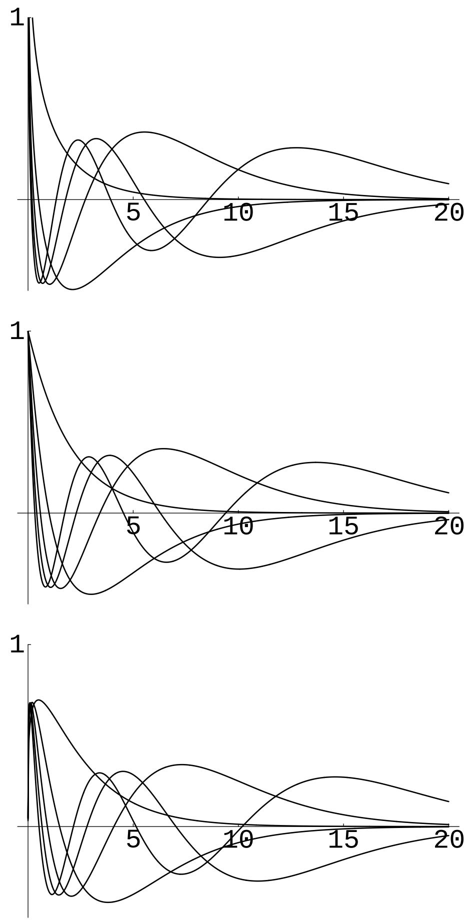

FIGURE 4: *Normalized eigenfunctions* $\psi_{n,a}(x)$ *with* $n = 0, 1, 2, 3, 4$. *At top* $a = -\frac{1}{2}$; *in the middle* $a = 0$; *at bottom* $a = +\frac{1}{2}$. *It is clear that in all cases* $\psi_{n,a}(\infty) = 0$, *but behavior in the limit* $x \downarrow 0$ *remains obscure: see Figure 5.*

$$\begin{aligned} &[\text{etc.}] \downarrow 0 \quad \text{as } x^{\frac{1}{2}} \text{ in the case } a = -\tfrac{1}{2} \\ &[\text{etc.}] \downarrow 0 \quad \text{as } x^{\frac{2}{2}} \text{ in the case } a = \quad 0 \\ &[\text{etc.}] \downarrow 0 \quad \text{as } x^{\frac{3}{2}} \text{ in the case } a = +\tfrac{1}{2} \end{aligned}$$

So the "surprising boundary conditions at the origin" do in fact appear to pose no physical problem. The situation is, however, more complicated than that ...as will soon emerge.

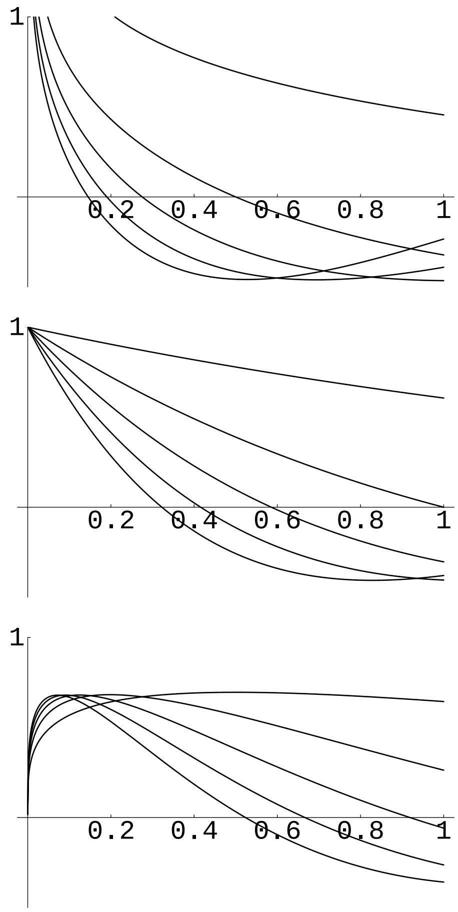

FIGURE 5: *Expanded view of Figure 4. As* $x \downarrow 0$ *the functions*

$$\begin{aligned} \psi_{n,-\frac{1}{2}}(x) &\to \infty \quad \textit{as } x^{-\frac{1}{4}} \\ \psi_{n,0}(x) &\to 1 \\ \psi_{n,+\frac{1}{2}}(x) &\to 0 \quad \textit{as } x^{+\frac{1}{4}} \end{aligned}$$

Matrix representation of the results in hand. Valuable insight can be gained from looking to the *matrix representation* of results achieved in preceding sections. We take as our point of departure the equation

$$\Big\{\big(\tfrac{1}{i}\tfrac{d}{dz}\big)z\big(\tfrac{1}{i}\tfrac{d}{dz}\big)+\tfrac{a^2}{4z}+\tfrac{1}{4}z-\tfrac{a}{2}\Big\}\psi_{n,a}=\big(n+\tfrac{1}{2}\big)\psi_{n,a} \tag{52}$$

obtained from multiplying (51) by $\frac{\hbar^2}{2m\ell^2}$ and writing $z = x/\ell$. All the labor is entrusted to *Mathematica*: we (see again (22)) define

$$\texttt{f[z\_,n\_,a\_]:=}\ \left[\frac{\texttt{Gamma[n+1]}}{\texttt{Gamma[n+1+a]}}\texttt{Exp[-z]z}^{\texttt{a}}\right]^{\frac{1}{2}}\texttt{LaguerreL[n,a,z]}$$

and examine expressions of the design

$$\mathbb{M}_a = \|M_{mn,a}\|$$
$$M_{mn,a} \equiv \int_0^\infty f[z,m,a]\,\mathsf{M}\,f[z,n,a]\,dz$$

in the cases $a = 0$, $a = \pm\frac{1}{2}$. The operators recommended to our attention by (52) are

$$\begin{array}{lcl} \mathsf{Q} \equiv -\partial_z z\,\partial_z & : & \text{QUADRATIC} \\ \mathsf{R} \equiv \frac{1}{4}z^{-1} & : & \text{RECIPROCAL} \\ \mathsf{L} \equiv \frac{1}{4}z & : & \text{LINEAR} \\ \mathsf{C} \equiv -\frac{1}{2} & : & \text{CONSTANT} \end{array}$$

In this notation $\mathsf{H}_a = \mathsf{Q} + a^2\mathsf{R} + \mathsf{L} + a\mathsf{C}$.

$$\boxed{\text{CASE } a = 0}$$

Using commands of the form

$$\int_0^\infty \texttt{Table[}$$
$$\texttt{Table[Simplify[-f[z,m,0]}\partial_z\texttt{(z}\,\partial_z\texttt{f[z,n,0])],\{n,0,4\}],\{m,0,4\}]dz}$$

we obtain

$$\mathbb{Q} = \frac{1}{4}\begin{pmatrix} 1 & 1 & 0 & 0 & 0 & \cdots \\ 1 & 3 & 2 & 0 & 0 & \cdots \\ 0 & 2 & 5 & 3 & 0 & \cdots \\ 0 & 0 & 3 & 7 & 4 & \cdots \\ 0 & 0 & 0 & 4 & 9 & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix}$$

$\mathbb{R} =$ undefined: matrix elements are non-convergent $\int$s

$$\mathbb{L} = \frac{1}{4}\begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 3 & -2 & 0 & 0 \\ 0 & -2 & 5 & -3 & 0 \\ 0 & 0 & -3 & 7 & -4 \\ 0 & 0 & 0 & -4 & 9 \end{pmatrix} \quad : \quad \ldots\text{s and } \vdots\text{s henceforth understood}$$

$$\mathbb{C} = -\tfrac{1}{2}\,\mathbb{I}$$

The implication is that

$$\mathbb{H}_0 = \mathbb{Q} + a^2\,\mathbb{R} + \mathbb{L} + a\,\mathbb{C}\Big|_{a=0} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{5}{2} & 0 & 0 \\ 0 & 0 & 0 & \frac{7}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{9}{2} \end{pmatrix}$$

which presents the familiar oscillator spectrum.

$\boxed{\text{CASE } a = +\tfrac{1}{2}}$

Matrix elements turn out to be of the form $\sqrt{\text{rational}}$. It is more instructive to display their numerical values: we compute

$$\mathbb{Q} = \begin{pmatrix} 0.250000 & 0.204124 & -0.091287 & -0.084515 & -0.079682 \\ 0.204124 & 0.750000 & 0.447214 & -0.103510 & -0.097590 \\ -0.091287 & 0.447214 & 1.250000 & 0.694365 & -0.109109 \\ -0.084515 & -0.103510 & 0.694365 & 1.750000 & 0.942809 \\ -0.079682 & -0.097590 & -0.109109 & 0.942809 & 2.250000 \end{pmatrix}$$

$$\mathbb{R} = \begin{pmatrix} 0.500000 & 0.408248 & 0.365148 & 0.338062 & 0.318628 \\ 0.408248 & 0.500000 & 0.447214 & 0.414039 & 0.390360 \\ 0.365148 & 0.447214 & 0.500000 & 0.462910 & 0.436436 \\ 0.338062 & 0.414039 & 0.462910 & 0.500000 & 0.471405 \\ 0.318728 & 0.390360 & 0.436436 & 0.471405 & 0.500000 \end{pmatrix}$$

$$\mathbb{L} = \begin{pmatrix} 0.375000 & -0.306186 & 0 & 0 & 0 \\ -0.306186 & 0.875000 & -0.559017 & 0 & 0 \\ 0 & -0.559017 & 1.375000 & -0.810093 & 0 \\ 0 & 0 & -0.810093 & 1.875000 & -1.060660 \\ 0 & 0 & 0 & -1.060660 & 2.375000 \end{pmatrix}$$

$$\mathbb{C} = \begin{pmatrix} -0.500000 & 0 & 0 & 0 & 0 \\ 0 & -0.500000 & 0 & 0 & 0 \\ 0 & 0 & -0.500000 & 0 & 0 \\ 0 & 0 & 0 & -0.500000 & 0 \\ 0 & 0 & 0 & 0 & -0.500000 \end{pmatrix}$$

The computed implication now is that

$$\mathbb{H}_{+\frac{1}{2}} = \mathbb{Q} + a^2\,\mathbb{R} + \mathbb{L} + a\,\mathbb{C}\Big|_{a=+\frac{1}{2}} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{5}{2} & 0 & 0 \\ 0 & 0 & 0 & \frac{7}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{9}{2} \end{pmatrix}$$

$\boxed{\text{CASE } a = -\tfrac{1}{2}}$

The situation becomes now more interesting: both $\mathbb{Q}$ and $\mathbb{R}$ are undefined, because the matrix elements in both cases are of the non-convergent form

$$\int_0^\infty e^{-z}\,\frac{\text{polynomial}}{z^{3/2}}\,dz$$

But if we construct

$$\mathbb{K} \equiv \mathbb{Q} + \left(-\tfrac{1}{2}\right)^2\mathbb{R}$$

we find that cancellations result in convergent integrals

$$\int_0^\infty e^{-z}\,\frac{\text{polynomial}}{z^{1/2}}\,dz$$

We obtain

$$\mathbb{K} = \tfrac{1}{4}\begin{pmatrix} \frac{1}{2} & \frac{\sqrt{1}}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{\sqrt{1}}{\sqrt{2}} & \frac{5}{2} & \frac{\sqrt{6}}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{\sqrt{6}}{\sqrt{2}} & \frac{9}{2} & \frac{\sqrt{15}}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{\sqrt{15}}{\sqrt{2}} & \frac{13}{2} & \frac{\sqrt{28}}{\sqrt{2}} \\ 0 & 0 & 0 & \frac{\sqrt{28}}{\sqrt{2}} & \frac{17}{2} \end{pmatrix}$$

$$\mathbb{L} = \tfrac{1}{4}\begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{1}}{\sqrt{2}} & 0 & 0 & 0 \\ -\frac{\sqrt{1}}{\sqrt{2}} & \frac{5}{2} & -\frac{\sqrt{6}}{\sqrt{2}} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{\sqrt{2}} & \frac{9}{2} & -\frac{\sqrt{15}}{\sqrt{2}} & 0 \\ 0 & 0 & -\frac{\sqrt{15}}{\sqrt{2}} & \frac{13}{2} & -\frac{\sqrt{28}}{\sqrt{2}} \\ 0 & 0 & 0 & -\frac{\sqrt{28}}{\sqrt{2}} & \frac{17}{2} \end{pmatrix}$$

$$\mathbb{C} = -\tfrac{1}{2}\mathbb{I}$$

The implication now is that

$$\mathbb{H}_{-\frac{1}{2}} = \mathbb{K} + \mathbb{L} + a\mathbb{C}\Big|_{a=-\frac{1}{2}} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{5}{2} & 0 & 0 \\ 0 & 0 & 0 & \frac{7}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{9}{2} \end{pmatrix}$$

$$\boxed{\text{CASE } a = +\tfrac{1}{2}, \text{ REVISITED}}$$

Thus motivated, we compute

$$\mathbb{K} = \tfrac{1}{4}\begin{pmatrix} \frac{3}{2} & \frac{\sqrt{3}}{\sqrt{2}} & 0 & 0 & 0 \\ \frac{\sqrt{3}}{\sqrt{2}} & \frac{7}{2} & \frac{\sqrt{10}}{\sqrt{2}} & 0 & 0 \\ 0 & \frac{\sqrt{10}}{\sqrt{2}} & \frac{11}{2} & \frac{\sqrt{21}}{\sqrt{2}} & 0 \\ 0 & 0 & \frac{\sqrt{21}}{\sqrt{2}} & \frac{15}{2} & \frac{\sqrt{36}}{\sqrt{2}} \\ 0 & 0 & 0 & \frac{\sqrt{36}}{\sqrt{2}} & \frac{19}{2} \end{pmatrix}$$

$$\mathbb{L} = \tfrac{1}{4}\begin{pmatrix} \frac{3}{2} & -\frac{\sqrt{3}}{\sqrt{2}} & 0 & 0 & 0 \\ -\frac{\sqrt{3}}{\sqrt{2}} & \frac{7}{2} & -\frac{\sqrt{10}}{\sqrt{2}} & 0 & 0 \\ 0 & -\frac{\sqrt{10}}{\sqrt{2}} & \frac{11}{2} & -\frac{\sqrt{21}}{\sqrt{2}} & 0 \\ 0 & 0 & -\frac{\sqrt{21}}{\sqrt{2}} & \frac{15}{2} & -\frac{\sqrt{36}}{\sqrt{2}} \\ 0 & 0 & 0 & -\frac{\sqrt{36}}{\sqrt{2}} & \frac{19}{2} \end{pmatrix}$$

$$\mathbb{C} = -\tfrac{1}{2}\mathbb{I}$$

which gives back the same result as before, but now more transparently:

$$\mathbb{H}_{+\frac{1}{2}} = \mathbb{K} + \mathbb{L} + a\mathbb{C}\Big|_{a=+\frac{1}{2}} = \begin{pmatrix} \frac{1}{2} & 0 & 0 & 0 & 0 \\ 0 & \frac{3}{2} & 0 & 0 & 0 \\ 0 & 0 & \frac{5}{2} & 0 & 0 \\ 0 & 0 & 0 & \frac{7}{2} & 0 \\ 0 & 0 & 0 & 0 & \frac{9}{2} \end{pmatrix}$$

The matrices displayed above are replete with patterns that I will not linger to describe explicitly. Each is manifestly hermitian (real symmetric).

The quantum theory of oscillators leads[30] to matrices

$$\mathbb{X} = \sqrt{\tfrac{1}{2}}\begin{pmatrix} 0 & +\sqrt{1} & 0 & 0 & 0 \\ \sqrt{1} & 0 & +\sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 & +\sqrt{3} & 0 \\ 0 & 0 & \sqrt{3} & 0 & +\sqrt{4} \\ 0 & 0 & 0 & \sqrt{4} & 0 \end{pmatrix}$$

$$\mathbb{P} = i\sqrt{\tfrac{1}{2}}\begin{pmatrix} 0 & -\sqrt{1} & 0 & 0 & 0 \\ \sqrt{1} & 0 & -\sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 & -\sqrt{3} & 0 \\ 0 & 0 & \sqrt{3} & 0 & -\sqrt{4} \\ 0 & 0 & 0 & \sqrt{4} & 0 \end{pmatrix}$$

which supply

$$\mathbb{X}^2 + \mathbb{P}^2 = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 & 0 \\ 0 & 0 & 5 & 0 & 0 \\ 0 & 0 & 0 & 7 & 0 \\ 0 & 0 & 0 & 0 & 5 \end{pmatrix}$$

$$\mathbb{X}\mathbb{P} - \mathbb{P}\mathbb{X} = i\begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & -4 \end{pmatrix}$$

The red elements are artifacts of the circumstance that we work here from *finite fragments* of ∞-dimensional matrices.

Whittaker draws essentially upon the Schrödinger representation[31]

$$\mathsf{p} = -i\partial_z$$

of the "momentum operator"—passing over without comment the fact that the latter is specific to *Cartesian* coordinates. Computation in the present context

[30] See ADVANCED QUANTUM TOPICS (2000), Chapter 0, page 24.
[31] I have here set $\hbar/\ell = 1$.

supplies in $\boxed{\textsc{case}\ a=0}$

$$\mathbb{X}=\begin{pmatrix} 1 & -1 & 0 & 0 & 0\\ -1 & 3 & -2 & 0 & 0\\ 0 & -2 & 5 & -3 & 0\\ 0 & 0 & -3 & 7 & -4\\ 0 & 0 & 0 & -4 & 9\end{pmatrix}$$

$$\mathbb{P}=i\begin{pmatrix} \frac{1}{2} & 1 & 1 & 1 & 1\\ 0 & \frac{1}{2} & 1 & 1 & 1\\ 0 & 0 & \frac{1}{2} & 1 & 1\\ 0 & 0 & 0 & \frac{1}{2} & 1\\ 0 & 0 & 0 & 0 & \frac{1}{2}\end{pmatrix} \quad : \quad \text{non-hermitian!}$$

Define

$$\tilde{\mathbb{P}}\equiv \text{hermitian part of } \mathbb{P}=i\tfrac{1}{2}\begin{pmatrix} 0 & 1 & 1 & 1 & 1\\ -1 & 0 & 1 & 1 & 1\\ -1 & -1 & 0 & 1 & 1\\ -1 & -1 & -1 & 0 & 1\\ -1 & -1 & -1 & -1 & 0\end{pmatrix}$$

and obtain

$$\mathbb{X}\tilde{\mathbb{P}}-\tilde{\mathbb{P}}\mathbb{X}=i\begin{pmatrix} 1 & 0 & 0 & 0 & -\frac{5}{2}\\ 0 & 1 & 0 & 0 & -\frac{5}{2}\\ 0 & 0 & 1 & 0 & -\frac{5}{2}\\ 0 & 0 & 0 & 1 & -\frac{5}{2}\\ -\frac{5}{2} & -\frac{5}{2} & -\frac{5}{2} & -\frac{5}{2} & -4\end{pmatrix}$$

In the $\boxed{\textsc{case}\ a=+\frac{1}{2}}$ we obtain

$$\mathbb{X}=\begin{pmatrix} 1.50000 & -1.22474 & 0 & 0 & 0\\ -1.22474 & 3.50000 & -2.23607 & 0 & 0\\ 0 & -2.23607 & 5.50000 & -3.24037 & 0\\ 0 & 0 & -3.24037 & 7.50000 & -4.24264\\ 0 & 0 & 0 & -4.24264 & 9.50000\end{pmatrix}$$

$$\mathbb{P}=i\begin{pmatrix} 0 & 0.40825 & 0.36515 & 0.33806 & 0.31873\\ -0.40825 & 0 & 0.44721 & 0.41404 & 0.39036\\ -0.36515 & -0.44721 & 0 & 0.46291 & 0.43644\\ -0.33806 & -0.41404 & -0.46291 & 0 & 0.47141\\ -0.31873 & -0.39036 & -0.43644 & -0.47141 & 0\end{pmatrix}$$

$$\mathbb{X}\mathbb{P}-\mathbb{P}\mathbb{X}=i\begin{pmatrix} 1 & \sim 10^{-16} & \sim 10^{-16} & \sim 10^{-16} & -1.59364\\ \sim 10^{-16} & 1 & \sim 10^{-16} & \sim 10^{-16} & -1.95180\\ \sim 10^{-16} & \sim 10^{-16} & 1 & \sim 10^{-16} & -2.18218\\ \sim 10^{-16} & \sim 10^{-16} & \sim 10^{-16} & 1 & -2.35702\\ -1.59364 & -1.95180 & -2.18218 & -2.35702 & -4\end{pmatrix}$$

Look finally to the $\boxed{\text{CASE } a = -\frac{1}{2}}$, where it is known already that

$$\mathbb{X} = \begin{pmatrix} \frac{1}{2} & -\frac{\sqrt{1}}{\sqrt{2}} & 0 & 0 & 0 \\ -\frac{\sqrt{1}}{\sqrt{2}} & \frac{5}{2} & -\frac{\sqrt{6}}{\sqrt{2}} & 0 & 0 \\ 0 & -\frac{\sqrt{6}}{\sqrt{2}} & \frac{9}{2} & -\frac{\sqrt{15}}{\sqrt{2}} & 0 \\ 0 & 0 & -\frac{\sqrt{15}}{\sqrt{2}} & \frac{13}{2} & -\frac{\sqrt{28}}{\sqrt{2}} \\ 0 & 0 & 0 & -\frac{\sqrt{28}}{\sqrt{2}} & \frac{17}{2} \end{pmatrix}$$

but where we discover that

$$\mathbb{P} \text{ is undefined}$$

because its matrix elements present integrals of the non-convergent design

$$\int_0^\infty e^{-z}\frac{\text{constant}}{z^{3/2}}dz + \text{non-pathological terms}$$

The discovered facts that

$$\mathbb{P} \text{ is } \begin{cases} \text{hermitian in the case } a = +\frac{1}{2}, \text{ but} \\ \underline{\text{non-hermitian}} \text{ in the case } a = 0 \text{ and} \\ \underline{\text{undefined}} \text{ in the case } a = -\frac{1}{2} \end{cases}$$

can be traced to the behavior of the wave functions $\psi_{n,a}(x)$ near the boundary point $x = 0$, as illustrated in Figure 5.

That Schödinger's $\mathsf{p} \equiv \frac{\hbar}{i}\partial_x$ is *<u>sometimes not self-adjoint</u> with respect to otherwise admissible wavefunctions* is an elementary fact, but a fact too seldom noted. The trivial argument: an integration-by-parts gives

$$\int_\alpha^\beta u^*(-i\partial_x v)\,dx = \int_\alpha^\beta (-i\partial_x u)^* v\,dx - i(u^*v)\Big|_\alpha^\beta$$

and

$$\text{self-adjointness requries } (u^*v)\Big|_\alpha^\beta = 0$$

In the context at hand (where we can drop the *'s) we however have

$$\psi_{m,a}(z)\psi_{n,a}(z)\Big|_0^\infty = -\psi_{m,a}(0)\psi_{n,a}(0) = \begin{cases} 0 & : \quad a = +\frac{1}{2} \\ 1 & : \quad a = 0 \\ \infty & : \quad a = -\frac{1}{2} \end{cases}$$

The problem here touched upon was taken up in the early/mid-1960s by physicists and mathematicians associated with Joseph Hirschfelder, a theoretical chemist who took his initial motivation from problems encountered in connection with his quantum theory of "hypervirial theorems."[32] The basic idea—approached in the literature from at least four different angles—is to adjust

$$\mathsf{p} \equiv -i\partial_x \quad \longmapsto \quad \tilde{\mathsf{p}} \equiv -i\partial_x + \lambda f(x)$$

and to assign to $f(x)$—assumed to be real-valued—such formal properties that it "surgically removes" the self-adjointness-destroying terms. In contexts such as those in which we presently find ourselves, Hirschfelder *et al* would have us write

$$\begin{aligned}\int_0^\infty u^*(-i\partial_x + \lambda f)\,v\,dx &= \int_0^\infty u^*(-i\partial_x v)\,dx + \lambda\int_0^\infty (u^*v)f\,dx\\ &= \int_0^\infty (-i\partial_x u)^*\,v\,dx + \underbrace{\lambda\int_0^\infty (u^*v)f\,dx + iu^*(0)v(0)}_{\text{require } = \lambda^*\int_0^\infty (u^*v)f\,dx}\end{aligned}$$

To achieve

$$(\lambda^* - \lambda)\int_0^\infty (u^*v)f\,dx = iu^*(0)v(0)$$

Hirschfelder sets

$$\lambda = -\tfrac{1}{2}i \quad \text{and} \quad f(x) = \delta_+(x) \equiv \lim_{\xi\downarrow 0}\delta(x-\xi)$$

The implication by $\psi_{m,0}(0)\psi_{n,0}(0) = 1$ (all m, n) is that in $\boxed{\text{CASE } a = 0}$ we should subtract

$$i\tfrac{1}{2}\begin{pmatrix}1&1&1&1&1\\1&1&1&1&1\\1&1&1&1&1\\1&1&1&1&1\\1&1&1&1&1\end{pmatrix}$$

from $\mathbb{P}$. But that is precisely the procedure (there called "extraction of the hermitian part") that on page 41 yielded $\tilde{\mathbb{P}}$.

[32] See Peter D. Robinson & Joseph O. Hirschfelder, "Generalized momentum operators in quantum mechanics," J. Math. Phys. **4**, 338 (1963); P. D. Robinson, "Integral forms for quantum-mechanical momentum operators," J. Math. Phys. **7**, 2060 (1966); A. M. Arthurs, "Momentum operators in quantum mechanics," PNAS **60**, 1105 (1968) [uses Feynman formalism to reproduce Hirschfelder's principal result]; Y. M. Chan & J. O. Hirschfelder, "Extending the domain of the Laplacian operator with the use of delta functions," PNAS **61**, 1 (1968). I pulled those papers from my dusty files, and have made no attempt to search the more recent literature.